



A framework for evaluating the sustainability of advanced powertrains

Walter Sweeting (2013)

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A framework for evaluating the sustainability of advanced powertrains

by

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ABSTRACT

Road vehicles represent a vital part of the world's mobility network. However significant concerns surrounding the energy supply and emissions associated with these vehicles have led to many alternative powertrains being proposed. Much research has been conducted evaluating how the in-use impacts of these compare to incumbent powertrains. This has shown that battery electric vehicles (BEV) have great potential to address many of the concerns, but assessments that go beyond the use phase suggest that changes in other stages, e.g. production, could abate these benefits.

The large battery packs of BEVs may incur substantial production impacts. However their reported impacts vary dramatically in the literature, which can introduce significant variations into whole life assessments of BEVs. To evaluate this uncertainty, a new life cycle assessment (LCA) for lithium-ion battery production and end-of-life processing was developed. This was combined with further models to permit studies of battery variables such as efficiency, lifetime, materials and specific energy, along with the trade-offs between them, on the whole life impacts of BEVs.

The inclusion of battery production impacts are vital in assessments of BEVs and can significantly alter the findings relative to incumbent vehicles. Different lithium-ion variants were shown to alter a BEVs lifetime impacts and to necessitate the normalisation of vehicle range to fully quantify their effects. A sensitivity analysis of the new battery LCA revealed less variability than in the current literature and indicated that assessments are hampered by limited production data, along with unrepresentative inventories for various specialist materials. Trade-offs between parameters may result in batteries with superior lifetimes only offering whole life CO_{2e} emissions reductions under limited scenarios when used in BEVs. The research also showed that for BEVs, increasing battery losses with power demands exacerbate the higher energy usage exhibited over many real-world driving situations compared to the European test cycle.

Overall this research has generated improved lifecycle models for lithium-ion batteries and incorporated many additional factors/scenarios to generate a framework that permits enhanced whole life sustainability assessments of alternative powertrains.

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LIST OF SYMBOLS AND ABBREVIATIONS

a	Acceleration (m/s^2)
A _v	Vehicle frontal area (m ²)
BatPaC	Battery Performance and Cost model (Developed by Argonne National Laboratory)
BEV	Battery electric vehicle (refers to vehicles solely powered by batteries)
B _i	Base mass percentages of non-cell components
BMS	Battery management system
C_{BEV}	BEV electricity consumption (kWh/km)
C _{cell}	Cell capacity (Ah)
C _d	Drag coefficient
CO _{2e}	Carbon dioxide equivalent emissions
C _{pack}	Pack capacity (Ah)
Cr	Coefficient of rolling resistance
DOD	Depth of discharge
e	Electron
E _{BEVP}	BEV emissions excluding those of the in-use electricity (g CO_{2e}/km)
E _{CV}	Whole life emissions from a vehicle substituted by a BEV (g CO_{2e} per km)
$\mathrm{E}_{\mathrm{grid}}$	Emissions from existing generation that could be replaced (g CO_{2e}/kWh)
E _{NC}	Emissions associated with new electricity generation (g CO _{2e} /kWh)
EoL	End-of-life
EV	Electric vehicle (refers to all EV systems e.g. BEVs and hybrids)
Fa	Force required for acceleration
F _{ad}	Aerodynamic drag force
F _{rr}	Rolling resistance force
G	Gravity (m/s ²)
GDP	Gross domestic product

GHG	Greenhouse gas
Ι	Current
ICE	Internal combustion engine
LCA	Life cycle assessment
LCI	Life cycle inventory
LCO	Lithium cobalt oxide (LiCoO ₂₎
LDV	Light duty vehicles (taken to encompass cars and light commercial vehicles)
LFP	Lithium iron phosphate
Li ₂ CO ₃	Lithium carbonate
LiPF ₆	Lithium hexafluorophosphate
LMO	Lithium manganese oxide
М	Mass (kg)
M_i	Molecular mass
Ν	Newton
n _e	Number of electrons
NEDC	New European Driving Cycle
NCM	Nickel cobalt manganese
NMP	N-methyl-2-pyrrolidone
NNC	Total non-cell mass percentage of battery pack
NOx	Nitrogen oxides
ρ	Density of air (kg/m ³)
Р	Power
PEM	Proton exchange membrane
PM	Particulate matter
PP	Polypropylene
PTFE	Polytetrafluoroethylene
PVC	Polyvinyl chloride

PVDF	Polyvinylidene fluoride
R _{cell}	Cell internal resistance
SO _{2e}	Sulphur dioxide equivalents emissions
SOC	State of charge
TTW	Tank-to-wheels (use phase)
V	Voltage
Ve	Velocity (m/s)
Vo	Open circuit voltage
VOC	Volatile organic compounds
WTT	Well-to-tank (fuel/energy production phase)
WTW	Well-to-wheels (fuel/energy production and use phases)

1. INTRODUCTION

1.1. Overview

Access to motorised transportation is one of the key factors that has enabled the development of the world we live in today. It is now integral to the operation of virtually all businesses, particularly in the developed world, and the economy as a whole. A reliable and affordable transportation system has also had a profound effect on people's expectations and opportunities, for example by increasing access to employment, leisure and educational facilities. This has resulted in many people becoming absolutely dependent on the current system.

Road vehicles have played a significant role in these changes and their numbers rapidly increased in the preceding century. This trend is set to continue (see Figure 1.1), with large demands expected from the developing world which, despite accounting for 85% of the global population in 2007, only contained a third of the world's car fleet (Pemberton, et al. 2009). The overall increases are expected to be dramatic, with the number of light duty vehicles (LDV) on the world''s roads set to double and sales treble by 2050.



(Constructed using data from Pemberton (2011), assuming a business as usual scenario) *Figure 1.1 Growth of the global population, number of vehicles, and LDVs sales*

However there are already significant problems related to the world"s current level of vehicles, e.g. energy demands, emissions and materials supply (see Section 1.2). These raise the questions:

- How can vehicles be adapted to improve their sustainability?
- Are the anticipated increases in the vehicle parc possible without severe detrimental effects?

In order to improve the overall sustainability of our current transport network, all modes and options, such as reductions in distances travelled and modal shifts e.g. from motorised personal vehicles to public transport or cycling, will need to be addressed. However, to permit sufficient analysis within the project timeframe, the focus of this work has been on LDVs, which create the greatest demands for materials and transportation fuel (WBCSD, 2004).

The following sections in this chapter firstly address some of the main issues that threaten the sustainability and expansion of our current vehicle fleet. Then, some of the powertrain options that could help mitigate these factors are briefly addressed, and finally the thesis as a whole is outlined.

1.2. Transportation challenges

This section highlights the extent of some of the problems facing LDVs. Two further concurrent issues, which are also linked with vehicle parc levels, are road safety and congestion. These are beyond the remit of this thesis, which has focused on the direct environmental impacts of LDVs. However, it is important to appreciate they may have implications on vehicles and repercussions on other factors. For example congestion leads to an exacerbation of emissions and higher safety expectations often incur additional material requirements.

1.2.1. Energy demand and supply

Oil supply

At present internal combustion engines almost exclusively propel the world's road vehicles. The majority of their energy is derived from crude oil, a finite resource, of which transport accounts for approximately 70% of demand (Kasseris and Heywood, 2007). The

upward trend in vehicles has therefore had a concomitant effect on oil demand, (Figure 1.2).



(Constructed using data from EIA (2011a) and EIA (2013))

Figure 1.2 Graph of approximate average annual oil price and supply

Future demand increases are expected to result mainly from transportation and projections suggest annual demand will reach 39-43 billion barrels by 2030, approximately a 1.4% annual increase (IEA, 2008; Kjärstad and Johnsson, 2009).

The supply and price of oil is however quite volatile, as shown in Figure 1.2, and significant concerns have been raised over potential supply issues and price hikes. These have previously caused major disruptions and contributed to increased inflation and unemployment (Hedenus, et al. 2010). Oil demand is also linked to gross domestic product (GDP). This link is weakening, due to higher oil prices and efficiency improvements, but it has been estimated that for every percentage increase in oil price, GDP is abated by 0.055% (IEA, 2008; Owen, et al. 2010).

There is presently a degree of uncertainty around oil reserves, with values depending not only on data accuracy, but also on what is deemed technologically and economically feasible to recover (which increases with oil price). Further discrepancies have also been suggested to result from intentional data manipulation to suit political or financial agendas (Laherrere, 2001). Values for "proven" oil reserves, which are those that should be recoverable from known reserves under existing economic conditions, have been given at 900 billion to over 1300 billion barrels (Owen, et al. 2010). However estimates of the ultimately recoverable reserves of conventional oil, which includes those only initially proven and yet to be discovered, are speculated to be in the region of 1 to 3 trillion barrels (IEA, 2008; Kjärstad and Johnsson, 2009).

There are also further significant unconventional oil reserves. Those suggested to be ultimately economic to extract could contribute an additional 2 to 3 trillion barrels of oil, 1 to 2 trillion from oil sand/extra-heavy oil and 1 trillion from oil shale (IEA, 2008). However their extraction will require large capital investment and production is more energy and emission intensive than for conventional sources. For example, petrol derived from tar sands is estimated to result in around 14% to 40% more lifetime greenhouse gas emissions and have over double the production costs (Arons, et al. 2007; Hughes and Rudolph, 2011).

To give a rough indication of how these different resources and potential demand increases could affect supply, Table 1.1 was constructed. This table presents two scenarios: the first assumed demand was curtailed at 2012 levels, while the second used an annual growth rate of 1.4% (see above). It was assumed extraction at a sufficient rate remained possible, which will become increasingly difficult as reserves dwindle and demand escalates, that is the problems of ,peak oil" are not accounted for.

Reserve source	Estimated	Estimated years reserves can meet demand	
	reserves (trillion	Assuming no	Assuming 1.4% per
	barrels)	demand increase	annum demand increase
Proven conventional	0.9-1.3	28-40	23-32
Total conventional	1.3-3	40-94	32-60
Total conventional and unconventional	3-6	94-188	60-92

Table 1.1 Estimated durations oil supply can meet demands using different sources

Further review on how much oil can be extracted at an acceptable financial and environmental cost is not possible here. However it is clear from Table 1.1 that current sources are limited and that if it were possible to halt the worlds escalating thirst for oil, by limiting the amount used by vehicles, significant long term supply gains are possible.

Global energy supply

Currently the world's total primary energy consumption is extremely unevenly spread amongst the population. Less than 3% is consumed by the poorest quarter, while nearly half is used by occupants of the G8 countries, which contain only 12% of the population (Armaroli and Balzani, 2011a). This indicates there is potential for huge increases in energy demand as the majority of the population approaches the energy intensive lifestyles of the wealthier nations. Projections suggest over a 50% increase between 2008 and 2035.

Over 80% of energy demand is met by natural gas, oil and coal. Like oil, natural gas and coal are finite resources. Estimates suggest that natural gas could be exhausted in 60 years, assuming demand remains constant at 2008 levels and using 2011 reserve estimates. Large amounts of natural gas are still being discovered though, which will help increase this duration, but demand is also anticipated to increase. Sufficient reserves of coal remain to meet current demands for over 100 years, but this could reduce substantially if historical increases are maintained (EIA, 2011b). Coal is a very carbon intensive fuel and increasing regulations and initiatives are being introduced to mitigate greenhouse gas emissions such as fitting carbon capture and storage technologies to coal power plants are receiving attention, but they increase the cost and reduce the efficiency of the plant, which will in turn increase resource demands (Hoffmann and Szklo, 2011).

The alternatives to these fossil sources are nuclear and renewables, which in 2008 accounted for approximately 15% of global energy demand (EIA, 2011b). Nuclear has the potential to allow significant increases in electricity production (Mackay, 2008). Safety risks surrounding nuclear power and the safe disposal of spent fuel, particularly following the Fukushima disaster in 2011, have however led to many nations limiting their nuclear energy ambitions, and in some cases prohibiting new construction altogether (Moriarty and Honnery, 2012; World Energy Council, 2012).

Potential exists to increase the amount of energy we source from renewables such as wind, tidal and solar. However, large increases to meet the majority of demands are expected to be problematic and costly for many nations (Mackay, 2008; Moriarty and Honnery, 2012).

1.2.2. Emissions issues

Air pollution

Air pollution is a significant problem, particularly in urban areas, with around 3,500 early deaths per year being attributed to poor air quality in the UK (HoC, 2009-10). The levels in some cities are now so dangerously high (see Figure 1.3), that their residents are being advised to stay indoors (The Guardian, 2013). This, coupled with predictions that without more ambitious environmental policies air pollution is set to become the top global environmental cause of premature deaths by 2050, makes increased action imperative (OECD, 2012).



(The Guardian, 2013)



Vehicles are a key contributor to air pollution, with various emissions being associated with both their use and production. Many of these are known to have a variety of both direct and indirect detrimental effects on human health and the ecosystem. Table 1.2 gives a brief overview of the most significant emissions, addressing their sources and effects. The potential health implications it highlights, such as increased breathing problems, mean emissions in populated areas are particularly hazardous due to the disproportionally high number of people affected. Vehicle tailpipe emissions, exacerbated by dense usage and congestion, are a main contributor to the localised high pollution concentrations currently found in many urban areas. This makes them an extremely important source to tackle.

The following sections address greenhouse gases (GHG) and the legislation surrounding emissions.

Emission	Source	Effects
Nitrogen	Transportation ≈30% (HoC,	Reacts to form nitric acid which contributes
oxides	2009-10). High combustion	to acid rain, lake acidification, and foliage
(NOx)	temperatures and pressures	loss. In the presence of VOCs, it can react to
	result in increased vehicle	form ozone. Exposure can affect the
	emissions.	respiratory system (Defra, 2010).
Sulphur	Sulphur in fuel, major	Reacts in the atmosphere to form sulphuric
dioxide	reductions have been	acid (see effects given for nitric acid from
(SO ₂)	achieved through regulations	NOx). Exposure constricts the airways and
	dictating low sulphur	presents particular problems for asthma
	contents.	sufferers (WHO, 2006).
Particulate	Transport, $\approx 18\%$. Brake and	Increased risks of lung cancer and
matter	tyre/road wear add to tailpipe	cardiovascular disease. UK anthropogenic
(PM)	emissions. Resuspension in	PM emissions, in 2005, were estimated to
	the air by traffic on roads is	reduce the average life expectancy by
	also a significant problem in	approximately 7 to 8 months. Abating
	some locations.	pollution levels are acting to lower figures,
		but no safe exposure level is suggested
		(Defra, 2010).
Ozone (O ₃)	Ozone is not a direct	It contributes to summer smogs, causes
	anthropogenic emission but	lung/breathing problems and affects plant
	results from reactions of	life, reducing growth, which has detrimental
	other pollutants, primarily	effects on arable crop yields (Defra, 2010).
	NOx and VOCs.	
Carbon	Incomplete combustion.	It is tasteless, odourless and poisonous. CO
monoxide		bonds to the haemoglobin in red blood cells
(CO)		in place of oxygen, leading to reduced
		oxygen levels (Mudakavi, 2010).
Volatile	Vaporisation of fuel and	Many suggested to be carcinogenic,
organic	vehicle emissions from	mutagenic or toxic and correlations shown
compounds	incomplete combustion.	between VOC levels and cancer rates
(VOC)		(Boeglin, et al. 2006; Khoder, 2007).

Table 1.2 Effects of vehicle emissions

Greenhouse gases

The greenhouse effect refers to the warming that results from atmospheric gases and clouds absorbing some of the infrared radiation emitted by the earth's surface and then reemitting it back down. The earth's surface emits more energy, on average, than it receives from the sun. Therefore, the greenhouse effect helps balance the energy the earth receives from the sun and emits to space, thereby creating approximate equilibrium. However additional GHG, e.g. carbon dioxide (CO_2) and methane in the atmosphere, also contribute to this effect. These subsequently alter the amount of infrared radiation reemitted back to earth, potentially leading to climate change (The Royal Society, 2010). When measuring GHG they are often reported in terms of carbon dioxide equivalents (CO_{2e}), were the relevant emissions are converted into the equivalent amounts of CO_2 needed to incur the same impacts, see Section 4.3.3.

When burned, the carbon locked in fossil fuels combines with oxygen to form carbon dioxide. This results in the vast quantities of fossil fuels now being consumed producing even larger quantities of CO_2 . For example over 3kg are produced for every one kg (approximately 1.3 litres) of petrol burned.

Correlations suggest that fossil fuel usage is the main cause of the exacerbated CO_2 concentrations in the atmosphere, observed since the mid 19th century, which are above any found in the last 800,000 years. Levels are now increasing by approximately half a per cent a year and similar trends have been observed for many other GHG (Stern, 2006; IPCC, 2007). In May 2013 recorded CO_2 levels reached 400PPM, which represents an increase of approximately 25% in only 50 years (Kunzig, 2013).

Predicting the effects of these increases is complex and speculative. A commonly concluded outcome is that if atmospheric concentrations of GHG were doubled, from preindustrial levels, the mean global temperature would be increased by approximately 3°C (Stern, 2006). This concentration of GHG is anticipated to be reached by 2050, if emissions levels are frozen at those of 2006, or by 2035 if recent increasing trends are maintained. Many scientists surmise that temperature increases above 2°C will have serious detrimental repercussions. To put this temperature increase into perspective, present day figures are only around 5°C higher than they were during the last ice age (Stern, 2006). Some of the main predicted outcomes of climate change are (Stern, 2006; The Royal Society, 2010):

- Precipitation becoming more unevenly spread between dry and wet regions.
- Increases in sea levels, potentially threatening the homes of 1 in 20 of the world"s inhabitants.
- Reduced crop yields, with Africa expected to be worst affected.
- Ocean acidification due to increased CO₂ concentrations.
- Mass extinction of possibly 15-40% of species with a 2°C temperature rise.

Further details on these and the many other consequences that have been suggested, are beyond the scope of this report, but can be found in reports such as Stern (2006) and IPCC (2007).

Legislation

In order to control the release of harmful emissions, many regulations are now in place that stipulate maximum permissible levels both in the air and from vehicles, for example the Euro emission test system (Council Regulation (EC) No 715/2007). Various schemes, such as the London low emission zone are also being implemented which place certain restrictions on vehicles in urban areas (HoC, 2009-10). Further details on many of the EU targets can be found in Defra (2010).

These regulations have had significant impacts, with UK air pollution reported to have halved compared to 1990 levels, despite a 20% increase in traffic. Unfortunately the rapid reductions achieved in the 1990s were seen to level off in the 2000s (HoC, 2009-10). Further restrictions on emissions, in line with the tightening of the Euro emissions standards implemented in the past, are now suspected not to be sufficient to meet future air quality targets (HoC, 2009-10).

Many further regulations are also being introduced to limit vehicle CO_2 emissions. The European Commission, for example, has now set targets for vehicle manufacturers average fleet emissions, with fines for non-compliance (Council Regulation (EC) No 443/2009). Figure 1.4 shows the average CO_2 emissions of vehicles sold in the UK up to 2012 and the proposed tightening of EU targets. The 2025 target is yet to be confirmed, but a preliminary range of 68-78 grams CO_2 /km has been suggested (Mock, 2013). The recent improvements, from 2007, indicate the trajectory needed to meet the forthcoming targets.

However, maintaining this rate of improvement will become increasingly challenging and in order to meet EU 2020 targets, either alternative powertrains or downsizing are expected to be necessitated (SMMT, 2013).



Figure 1.4 Historical vehicle CO₂ emissions and proposed EU targets

The majority of the current legislation however focuses on the in-use impacts of vehicles (specifically the tank-to-wheels (TTW) phase), which creates the potential for problem shifting to other phases, e.g. those of vehicle and fuel production.

1.2.3. Vehicle production and disposal

The projected number of vehicles, shown in Figure 1.1, will require vast amounts of materials for their production and maintenance, which will subsequently need to be dealt with at their end-of-life. Figure 1.5 indicates that, based on fixed vehicle and aftermarket/production process waste masses of 1190kg and 620kg respectively (Winfield, et al. 2007), over 10 billion tonnes of materials will be involved in the whole life of the world"s LDV fleet between 2010 and 2050. These wastes will occur at different times throughout a vehicle"s life, but in the figure they have all been attributed to the year in which it was produced.

There are concerns over the increasing impacts and difficulties of further materials extraction, as lower grade and more inaccessible deposits need to be exploited to meet demands. This, coupled with the fact some materials are now regarded as critical, means the efficient use and recycling of vehicle materials will play an important role in their long term sustainability (European Commission, 2010; Allwood, et al. 2011).



Figure 1.5 Vehicle lifecycle wastes

The majority of the problems associated with vehicles are generally attributed to their inuse phase, but their production impacts also present issues (Lane, 2006; Volkswagen AG, 2008). The relative importance of these problems is anticipated to significantly increase with the advent of alternative powertrains. This will result not only from lower in-use impacts, but also from alternative powertrain components, such as batteries and fuel cells. These components can represent a significant part of a vehicle''s mass, and often have large impacts associated with their materials and production processes (Notter, et al. 2010).

1.2.4. Summary

Current crude oil reserves could be exhausted in a few decades and although further reserves could be exploited, they will only be temporary measures and bring with them undesirable consequences. Additional constraints on other forms of energy mean that, in order to improve the long-term sustainability of LDVs, not only will alternative fuels be necessitated, but their total usage will need to be abated.

The detrimental influences of current vehicle emissions have led to a raft of legislation, which is anticipated to make it increasingly difficult for conventional vehicles to meet required targets. This, coupled with energy constraints, suggest that powertrain alterations will be unavoidable in the future.

Materials supply and production issues have the potential to impact on future powertrain choices, with materials such as rare earth and platinum group metals, which are utilised in motors and fuel cells respectively, being listed as critical (European Commission, 2010).

1.3. Advanced Powertrains

Conventional internal combustion engine powertrains waste the majority of the energy they consume. Figure 1.6 depicts how the energy used by an efficient modern diesel vehicle is utilised. This shows that there is significant potential to reduce the LDV fleets energy usage.



Figure 1.6 Factors accounting for the energy consumption of a diesel vehicle

Several alternative powertrains and fuels could be employed in vehicles to mitigate energy usage and some of the other issues discussed in Section 1.2, but all have their respective drawbacks. The main benefits and problems associated with some of these options are given in Table 1.3 and a more thorough assessment is included in Chapter 2.

All the options given in Table 1.3, or combinations of them, may form part of the future LDV fleet. However, it indicates battery electric vehicles (BEV) have the greatest potential to minimise energy consumption and can eradicate tailpipe emissions. This, along with the further benefits that the infrastructure for their fuel, i.e. electricity, already exists to some extent and that it can be produced from a variety of renewable sources have resulted in BEVs becoming the focus of this research.

Powertrain/	Benefits	Drawbacks
fuel		
Advanced	Mature technology, cost and	Dependent on oil supply, emissions and
petrol/diesel	existing fuel infrastructure.	meeting future emissions regulations
engines		will become increasingly difficult.
Conventional	Only relatively minor	Tailpipe emissions. May only be able to
engines using	changes to conventional	meet a fraction of demand without
biofuels	vehicles needed, increased	creating major further problems, e.g.
	sustainability and can reduce	land-use change and competition with
	emissions.	other crops (Bindraban, et al. 2009; Di
		Lucia, et al. 2012).
Hydrogen	Zero tailpipe emissions and	Overall emissions benefits dependent on
fuel cells	can use a variety of primary	fuel production route, high cost,
	energy sources.	requires new fuelling infrastructure,
		may utilise scarce materials and
		possible high total energy requirements.
Battery	Zero tailpipe emissions,	Overall emissions and energy benefits
electric	variety of primary fuel	dependent on fuel production route,
vehicles	sources and have the greatest	high vehicle costs, limited ranges, may
	potential to minimise energy	utilise scarce materials and long
	usage (Messagie, et al. 2010).	recharge times.

Table 1.3 Benefits and problems associated with several powertrain options

1.4. Research aim and objectives

1.4.1. Preamble

This section provides a summary of the key findings from the literature review, detailed above and in Chapters 2 to 3, which were used to identify the focus of the research performed in this thesis.

The above sections highlighted the challenges facing the world"s current LDV fleet, which will be exacerbated by large anticipated demand increases unless substantial action is taken. These considerations have led to increasing legislation which has put pressure on manufacturers to improve their vehicles. Further legislation is also envisaged which will make the use of conventional internal combustion powertrains and fuels increasingly unviable. This showed that there is an urgent need for alternative vehicles.

Many alternative powertrains and fuels, for example biofuels, hydrogen and electricity, have been proposed to help address these challenges, each offering specific advantages and disadvantages. Significant research has been conducted which has investigated the use and fuel production impacts associated with these alternatives. For example, the source of the electricity used to power BEVs (Doucette and McCulloch, 2011). This research has typically aimed at providing comparisons with incumbent vehicles and has shown that out of the alternative powertrains currently proposed, BEVs have the greatest potential to help address the transportation problems of energy demand and emissions.

There are however various factors that can affect the findings of such comparisons, many of which are complicated when alternative powertrains are involved. Vehicle in-use impacts are dependent upon how it is used and driven. Standard driving cycles are typically used to model the in-use phase of vehicles and the discrepancies these can introduce, against those found in the real-world, are well known for conventional vehicles (Samuel, et al. 2005; Transport and Environment, 2013). However, simulations and test data have shown the energy consumption of BEVs may be even more variable than their conventional counterparts. For example, energy consumption increased by over 70% when large auxiliary draws, such as those from cockpit heating and demisters were modelled. When considering the standard European test is performed with such unessential auxiliaries switched off, this could lead to exaggerated discrepancies for some alternative powertrains (Commission Regulation No 101; Sweeting, et al. 2011).

Non-powertrain factors, e.g. the coefficient of drag, also influence a vehicle"s in-use impacts. Vehicles fitted with alternative powertrains are typically designed with efficiency high on the agenda. This often means that their non-powertrain parameters are more optimised than those of vehicles fitted with conventional powertrains. This can create problems with comparisons between actual vehicles featuring alternative and conventional powertrains, because it can be unclear what differences arise from other factors.

A further significant issue, surrounding the benefits of alternative vehicles and the results of comparisons, is their production/end-of-life (EoL) impacts. These are often overlooked with the in-use phase being the focus of existing research and legislation, potentially leading to problem shifting to these phases. Some assessments have now also incorporated the production phase of vehicles, which results in a narrowing of the reported differences

between many alternative powertrains and incumbent versions (Notter, et al. 2010; Ma, et al. 2012). The results of such assessments are however highly variable, being dependent upon many assumptions. Some of these variables e.g. lifetime distance travelled, are discussed in a few assessments (Notter, et al. 2010; Hawkins, et al. 2013), but many, particularly the secondary effects emanating from the choices of new technologies, have received far less attention. Taking the choice of a battery for an electric vehicle as an example, some of the variables which could affect the assessment are:

- The lifetime of the battery.
- The battery specific energy and power.
- The battery efficiency.
- The accuracy and assumptions use to model the production impacts.

These variables will involve trade-offs with one another and with other phases in the vehicles lifetime. For example, would a battery that offers longer life but lower specific energy be advantageous?

Quantifying the many potential variables amongst powertrains, establishing their importance and identifying optimal choices is therefore complex due to the interplays between factors and trade-offs they necessitate.

The batteries of electric vehicles were identified as a particular problem in assessments due to the above variables coupled with their large mass, which will affect in-use energy consumption and potentially result in large production/EoL impacts. Due to the relatively high energies, powers and efficiencies lithium-ion batteries offer, compared to other options, they are anticipated to be the staple choice for BEVs in the coming years.

Further investigation showed limited LCA data was available on the production of lithiumion batteries in the existing literature. The assessments that were identified showed their production may incur significant impacts. However, the reported findings varied to such a degree that they could substantially affect the overall results of whole life BEV assessments. Assessments which also covered the EoL of lithium-ion batteries were found to be even more limited, with the impacts often being excluded or only partly addressed in the identified production LCAs. Great variation amongst lithium-ion batteries, e.g. specific energy and lifetime were also reported, which will also affect the impacts from all phases of a BEV"s lifetime.

1.4.2. Research rationale

The literature review, summarised above, identified several areas where limited data or inconsistencies in existing research have introduced significant variability into LCAs of alternative powertrains. Specifically the key weaknesses identified were:

- Limited and highly variable data regarding the production impacts of lithium-ion batteries. This variability was found to substantially affect the reported whole life impacts of BEVs and comparisons with other powertrains.
- The general omission or only partial assessment of EoL impacts in lithium-ion battery LCAs.
- Variability between the assumptions, e.g. vehicle characteristics and life cycle inventory data, used in assessments of alternative powertrains.
- A deficiency of assessments which compare the full effects of battery parameters and different lithium-ion variants under consistent assumptions on the whole life impacts of BEVs.
- A lack of research concerning the combined effects of battery parameters, the production/EoL phases and the trade-offs between them on BEV whole life impacts.

From these findings evaluation of the whole life impacts of BEVs, fitted with lithium-ion battery packs, was identified as an imported area where further research was required. This area, and more specifically the variations emanating from the production, EoL and differing parameters of their battery packs, subsequently became the focus of this research.

To study the variations caused by both differences in production impacts and parameters, three different lithium-ion battery chemistries were selected for evaluation based on their cathode materials. These were lithium iron phosphate (LFP), lithium manganese oxide (LMO) and lithium nickel cobalt manganese (NCM), which were identified as currently being the most feasible options for BEVs (see Section 2.3.2).

Based on the identified existing limitations and above focus, the research hypothesis, aim and objectives were derived.

1.4.3. Hypothesis

Limited evaluations of some phases, variables and trade-offs, in existing assessments of vehicles using alternative powertrains, have led to potential discrepancies between their predicted impacts and those that actually result during their whole life. Inclusion of these factors was postulated to show that additional research regarding the parameters, production and use of components employed by alternative powertrains is necessary. These should either, ensure that the suggested results of a particular powertrain choice are justifiable throughout the vehicles lifecycle, or highlight the degree of variability they introduce.

The hypothesis of this thesis was therefore that:

"In order to improve the results of powertrain assessments, more holistic frameworks are needed, which identify and incorporate the additional important variables and trade-offs involved".

1.4.4. Research aim

The overall aim of the research was to quantify the effects of variables resulting from electric vehicle batteries and develop a framework that permits enhanced parametric assessments of the whole life impacts and implications of BEVs, thereby enabling more holistic assessments of their sustainability.
1.4.5. Objectives

The main objectives of the research were to:

- 1. Undertake a life cycle assessment (LCA) of lithium-ion battery production, to enable investigations of the large discrepancies found amongst existing assessments and how variations in the chemistry affect the results.
- 2. Identify potentially significant variables or assumptions in battery production LCAs and evaluate their potential effects on the results.
- 3. Investigate the EoL impacts of lithium-ion batteries and expand the production LCA to incorporate their effects on the whole pack.
- 4. Integrate the battery LCA into a whole life vehicle model which enables the effects of battery production and EoL impacts on a BEV's lifetime to be assessed.
- 5. Evaluate how battery parameters can influence the lifetime impacts of BEVs. The additional parameters considered were:
 - Battery lifetime.
 - Battery specific energy.
 - Battery energy efficiency.
- 6. Quantify the effects of trade-offs between battery parameters, production/recycling and in-use impacts.
- 7. Use life cycle analysis to evaluate the whole life sustainability of BEVs, provide comparison with an efficient ICE vehicle and develop an outline framework for conducting more holistic impact assessments.

1.5. Main thesis contributions

The research generated improved life cycle assessments of electric vehicle batteries and quantified the effects of many of their variables on the whole life sustainability of BEVs. This research culminated in the generation of an outline framework that provided an enhanced methodology for sustainability assessments of alternative powertrains.

The thesis is further supplemented by additional novel data generated from work in the surrounding areas. These included studies on the factors affecting BEV energy usage and how fuel taxation could impact on the economics of alternative powertrains. Further details on these areas were presented in research papers by the author, Sweeting, et al. (2011) and Sweeting and Winfield (2012), respectively (see Appendix A).

A major part of the thesis was the development of a new life cycle assessment for lithiumion batteries. This was subsequently integrated into a whole vehicle model, which fed into the framework. This assessment helped establish the reasons for the large variations in current battery LCAs and builds on existing knowledge by:

- Incorporating the effects of battery production, EoL, efficiency, specific energy and lifetime, into a single assessment which enabled their combined impacts on the whole vehicle cycle to be studied. These parameters are typically only evaluated on their own, in subsets or at the battery level. For example, assessments which focus on battery LCA have typically used fixed values or very simple estimates for the in-use phase and battery efficiency models have tended to only address individual cells (e.g. they do not consider production or the effects on the devices they are used in). To achieve these studies, works on vehicle and battery modelling were used to construct an in-use model, which was subsequently brought together with the battery LCA. This enabled data to be generated, which helped to identify optimal trade-offs that could minimise the whole life impacts of BEVs.
- Allowing the influences of several different lithium-ion chemistries to be evaluated under consistent assumptions.
- Addressing some of the discrepancies found between the inventories in current LCAs and those of actual processes and batteries. For example, the mass percentage of cells incorporated in the battery pack was adjusted to be more representative of those in current BEVs and new production inventories for many key materials and processes were derived.
- Incorporating the recycling impacts of the entire battery pack.

Overall the research and final framework facilitated more holistic assessments of the sustainability of BEVs, by highlighting the potential direct and indirect impact variations resulting from some often overlooked factors. This should subsequently help avoid problem shifting and enable benefits to be maximised.

1.6. Outline of thesis

The overall research plan followed in this thesis is shown in Figure 1.7.



Figure 1.7 Research flow chart

How each of the stages, shown in Figure 1.7, built to fulfil the overall objectives of the research is outlined below:

- (1) The initial research, given in the first part of this Chapter, outlined the problems associated with current road vehicles. This provided the basis as to why research into establishing the whole life impacts of alternative powertrains was needed.
- (2) The literature review in Chapter 2 evaluated the sustainability of the main alternative powertrains proposed and how other vehicle parameters can also affect vehicle impacts. This allowed the research to be focused on the option with the greatest potential and showed how discrepancies in other aspects can affect the results of vehicle LCAs.
- (3) Due to BEVs being identified as having the greatest potential to mitigate vehicle energy use and emissions, the latter part of Chapter 2 further investigated their batteries. This stage reviewed the problems associated with current vehicle traction batteries and the potential of future chemistries. The results identified the most important battery variables, which will affect the impacts of BEVs, and the chemistries expected to be used in the coming years. These findings fed into the subsequent assessment which studied there effects.
- (4) This stage formed a further part of Chapter 2 and entailed an investigation of lithium-ion battery EoL options. This identified the most promising route and provided background data to help during the construction of the recycling LCA.
- (5) The literature review, presented in Chapter 3, examined the life cycle approach for assessing vehicles and reviewed existing assessments. This was complemented by a secondment to Tata Steel"s environmental department, in order to gain first-hand experience on LCA methodologies and specialist software from industry experts. This review identified significant variations in lithium-ion battery LCAs, which led to a specific focus on identifying their drawbacks, limitations and discrepancies.
- (6) This stage, given in Chapter 4, involved the development of a new LCA for lithium-ion batteries, which was used to identify significant processes, materials and assumptions. The model was parameterised to allow the effects of three different lithium-ion chemistries and key factors to be studied. Together with the findings from the literature review and the model results, presented in Chapter 6, this stage helped fulfil objectives 1 and 2 of this thesis.

- (7) The latter part of Chapter 4 developed the production LCA to incorporate the EoL phase. This enabled generation of data on the end-of-life phase of lithium-ion batteries, given in Chapter 6, which covered objective 3.
- (8) In Chapter 5 the battery LCA was integrated with further assessments for the remainder of the vehicle, use and maintenance phases, to create a whole life vehicle model. This Chapter also included the development of a conventional diesel vehicle model for use in comparisons. The use phase assessment was constructed to permit factors, such as the coefficient of drag, to be matched to trial vehicles and also to model battery parameters. For example energy efficiency and specific energy. This enabled the effects of the battery parameters on the use phase to be quantified. To supplement and verify the in-use values derived, trials were conducted using a BEV to provide data for real-world energy consumptions.
- (9) This stage used the whole life model to, quantify the impacts of batteries on the lifetime of BEVs, study how variables will affect the results, provide comparisons with a conventional vehicle and investigate trade-offs between parameters. The findings are presented and discussed in Chapter 7. Together with the previous stage, this covered objectives 4 to 6 and the first part of 7.
- (10) The conclusions, Chapter 8, summarised the findings, highlighted the research contributions and provided an outline framework for assessing the sustainability of alternative powertrains. This concluded objective 7.

Stages 7 to 10 (Figure 1.7), were performed iteratively. This permitted potentially significant factors, identified in the preliminary findings, to be adjusted or added to the LCA model.

2. REVIEW OF VEHICLE TECHNOLOGIES

This chapter provides a brief review of the main vehicle technologies proposed to help address some of the transportation challenges examined in Chapter 1. The first section addresses the potential of various alternative powertrains, while the second investigates how other vehicle factors, such as mass reduction, can provide improvements and affect the results of vehicle comparisons. The final section provides a more in-depth review of batteries for electric vehicles, due to their importance in the overall thesis.

2.1. Advanced powertrains and fuels

In order to help identify optimal choices which could achieve the greatest improvements, in the context of sustainable vehicles, it is important to appreciate the potential and pitfalls of all the key powertrains which could be utilised. This section therefore briefly reviews the main alternative powertrains and fuels, to evaluate their potential to reduce energy consumption and emissions.

2.1.1. Advanced internal combustion engines

In 2007 The King Review of low-carbon cars, concluded that CO_2 reductions of up to 30% could be achieved through the use of new technologies on internal combustion engine (ICE) vehicles (King, 2007).

The main technologies suggested to achieve these reductions, such as direct injection, engine downsizing, variable valve timing and turbocharging, are now being implemented on mainstream engines, such as Ford's EcoBoost petrol unit, fitted to the new Fiesta and Focus models (Ford Motor Company, 2013). In the 5 years from 2007 these changes, along with increased numbers of diesel and some alternatively fuelled vehicles, have achieved a 20% CO_2 reduction in average new UK car emissions. Further improvements are anticipated. However, in order to meet future targets major alterations such as hybridisation are suggested to be necessitated (Berggren and Magnusson, 2012; SMMT, 2013). Furthermore, as concluded by King (2007), in order to achieve long term decarbonisation goals, a powertrain utilising a carbon-free fuel will be the only solution.

Levels of other ICE vehicle emissions, such as NOx and carbon monoxide have also been significantly reduced. However, real-world in-use emissions of some of these gasses are still frequently above those stipulated in standards and achieved under defined laboratory type approval tests (Samuel, et al. 2005; Weiss, et al. 2012).

2.1.2. Alternative fuels

Common biofuel sources are currently rapeseed, which is used to produce biodiesel, and sugar cane or maize used to produce ethanol, a petrol substitute.

Biofuels are already being extensively used throughout the world. Since 2008 The Renewable Transport Fuel Obligations Order (2007), has stipulated that major suppliers of hydrocarbon oils to the UK have to also supply renewable fuels for road vehicle use. The amounts set were >2.56% by volume of the hydrocarbon oils they supplied, with annual rises to 5% in 2013, reduced from 5.26% by The Renewable Transport Fuel Obligations (Amendment) Order (2013). Similar trends are found in other countries, to meet regulations such as the EU Renewable Energy Directive (Council Directive 2009/28/EC).

Most engines require no alterations for 5 to 10% biofuel blends, but above this relatively inexpensive modifications are often required (King, 2007). Biofuel blends can affect vehicle emissions, for example potentially increasing NO_X and VOC levels, (Defra, 2010). The energy densities of biofuels also tend to be lower than conventional fuels, meaning larger volumes are necessitated for equivalent vehicle ranges. For example, petrol containing 5% and 15% ethanol would only contain approximately 98% and 95% respectively, of the energy in the equivalent volume of fossil fuel petrol (JEC, 2011a).

Biofuel production

Biofuel production has increased rapidly in recent years, with biodiesel output in the European Union (EU) reported to have expanded by over ten-fold in the decade up to 2009 (Nuffield Council on Bioethics, 2011). Policies such as the European Commission''s Renewable Energy Directive, which stipulates at least 10% of transportation energy must come from renewable sources by 2020, are a major driver behind this expansion (Council Directive 2009/28/EC). This rapid expansion however has resulted in many negative effects being attributed to biofuels. Some of the most significant are:

• Land use change. This can either be direct or indirect, where land previously used for food crops is used for biofuels, subsequently requiring additional land to be found for the displaced food crops. The loss of forest land results in the release of large amounts of GHGs. It has been calculated that if current biofuels are grown on cleared forest land, between 60 and 270 years of growth will be required before their emissions savings offset those released during the initial land use change (King, 2007).

- Competition with food crops, possibly leading to price increases, shortages or security issues.
- Loss of ecosystems and biodiversity, resulting from both land conversion and increased use of pesticides.
- Increased eutrophication, resulting from the use of fertilizers (Nuffield Council on Bioethics, 2011; Di Lucia, et al. 2012).

The production, and therefore supply, of biofuels is also at the mercy of many external factors, for example pests, disease, drought and floods (King, 2007).

These factors have led to the relaxing of targets involving biofuels (DFT, 2013; The Renewable Transport Fuel Obligations (Amendment) Order, 2013).

The growth of biofuels absorbs CO_2 , which can offset that emitted during their combustion. However there are many other phases during their lifetime that will result in uncompensated emissions, as shown in Figure 2.1. These considerations result in biofuels being far from carbon neutral and are further exacerbated by any emissions from land use change (Council Directive 2009/28/EC).



Figure 2.1 Emissions associated with biofuel production

Biofuels can also be produced from wastes. This option has the advantage of eradicating the issues given above regarding crop growth. However, they would still require processing, supplies are limited and commercial scale systems would often require amassing inputs from a large area (JEC, 2001b).

2.1.3. Fuel cells and their fuel

Several different types of hydrogen fuel cell exist. However, this section focuses on the proton exchange membrane (PEM), which is presently the most suitable for automotive applications (Campanari, et al. 2009). Fuel cells are incorporated into powertrains similar to those in BEVs, see Section 2.1.4, in place of the main battery pack. An additional energy store, often a small battery pack, is also typically included. This improves the system efficiency, absorbs energy from regenerative braking and helps the fuel cell deal with transient loads (Thounthong and Davat, 2008).

A basic hydrogen PEM fuel cell consists of an exchange membrane layer sandwiched between porous electrodes. Hydrogen and oxygen are fed to the electrodes, the anode and cathode respectively, where they react to form water and produce a current.

In order for a fuel cell to operate effectively, particularly in larger units like those required for automotive propulsion, many auxiliaries are necessitated. For example, heating/cooling systems, air pumps, humidifiers, valves and converters to manipulate the output power (Larminie and Dicks, 2003). All these parts add to the cost, complexity, size and weight of a fuel cell system.

Efficiencies are dependent on the power draw from the cell, decreasing as the draw increases and upon the composition of the feed fuel. However, typical efficiency values for hydrogen fuel cells lie between 45-65%, with the balance being dissipated as heat (Campanari, et al. 2009; Armaroli and Balzani, 2011b).

Along with the development and efficiency of hydrogen fuel cells, there are two further key issues, the production and storage of hydrogen. These are discussed in the following subsections.

Hydrogen production

Pure hydrogen is not a natural resource. It must be produced from hydrogen rich fuels such as crude oil, coal, gas and biomass or via electrolysis of water (King, 2007). Therefore, it is only a means of storing energy and not an alternative primary fuel supply.

Over 95% of hydrogen is currently derived from fossil fuels, with steam reforming of natural gas being the largest contributor (Armaroli and Balzani, 2011b). Contaminants e.g. sulphur and carbon monoxide, in the output hydrogen can severely affect PEM fuel cells. This incurs further processing to ensure contaminants in the fuel are below harmful levels

(Larminie and Dicks, 2003). Efficiencies for natural gas steam reforming are around 80% (Campanari, et al. 2009).

Water electrolysis can yield very pure hydrogen. However it is a far more expensive method than steam reforming. Electrolysers are around 70-80% efficient, but they require DC power which incurs additional losses when inverted from AC supplies (Armaroli and Balzani, 2011b).

Hydrogen storage

Hydrogen is far more difficult to store than current automotive fuels. These difficulties arise from the unique properties of hydrogen and create several issues:

- The density of hydrogen is extremely low, 84 grams per m³ at atmospheric pressure and 20°C, approximately 9000 times lower than petrol"s. To store sufficient quantities of energy on-board a vehicle the density must therefore be increased significantly.
- Leakage rates. The low density, along with the fact hydrogen molecules are very small and have high average velocities, result in it not only being able to seep out of minuscule openings, but also doing so at rates higher than other gases.
- Diffusion into materials. The same properties which cause hydrogen to leak so readily also enable it to diffuse into many materials. This diffusion can have detrimental effects on the material properties, for example by inducing cracking. The materials used for transmission and storage must therefore be carefully selected.
- Safety. Overall the safety implications of hydrogen are not thought to be worse than those of many current fuels (Markert, et al. 2007). However additional safety issues result from the storage methods used (see Table 2.1).

Several different methods can be used to increase the density of hydrogen. The main options, together with their advantages and disadvantages are summarised in Table 2.1. This shows they all have significant drawbacks and will increase the overall energy demand of a hydrogen fuelled vehicle. The various components needed to hold and release the hydrogen (e.g. pressure vessels and heat exchangers) will also add to the system mass, volume, cost and complexity (Ahluwalia, et al. 2012).

Method	Advantages	Disadvantages
Liquefaction	Density increased to	Requires cooling to 20K, which uses 30-40% of
	71kg/m ³ , but this still	the energy content.
	only gives an energy	Evaporation - losses of 1-5% per day are
	density of around a	anticipated, with the problem becoming more
	quarter of petrol"s.	acute the smaller the stored volume.
	Relatively low pressure.	Air in the system may result in explosive
		mixtures.
Compressed	Simplest method.	Pressurisation requires around 10-15% of the
gas	No losses under normal	energy content.
	conditions.	Very high pressures (typically 350-700bar).
		Diffusion into the container materials.
		Low energy density $\approx 15\%$ of petrol"s.
Reversible	Low pressure.	Low efficiency due to the heat released during
metal	Less volume required	recharging reactions or consumed during the H ₂
hydrides	than compression.	release phase.
	Reformers not required.	Cycle life/durability requires further testing.
H ₂ rich fuel	Fast refuelling.	Many compounds do not readily release H ₂ .
e.g. sodium	Storage, often at	Reactions produce by-products, many of which
borohydride	atmospheric temperature	are hazardous and must be safely removed and
which reacts	and pressure.	treated.
with water to	The release of hydrogen	Compounds are energy intensive and expensive
produce H ₂ .	can often be controlled.	to produce.

(Larminie and Dicks, 2003; Satyapal, et al. 2007; Armaroli and Balzani, 2011b; Ahluwalia, et al. 2012)

Table 2.1 Pros and cons of various hydrogen storage methods

A further option is on-board reforming. This has the advantages of removing the need to store hydrogen, quick refuelling and potentially being able to use existing fuels e.g. petrol, and their associated infrastructure. However, on-board reformers will bring vehicle penalties such as increased mass, lower efficiencies and in-use emissions (Campanari, et al. 2009).

2.1.4. Battery powered electric vehicles

Several different electric vehicle architectures exist, for example hybrids and plug-in hybrids. These main categories also vary e.g. series or parallel hybrids, along with the energy source e.g. batteries, super capacitors or flywheels (Chan, 2002). The components and energy flows for three common configurations are shown in Figure 2.2.



Figure 2.2 Electric vehicle architectures

The components already incorporated in electric vehicles, e.g. traction motors and batteries, can also be used to provide regenerative braking. This enables some of the energy usually dissipated as heat during braking to be recouped, thereby lowering energy consumption.

Hybrids can offer efficiency improvements over conventional vehicles, however they do not eradicate the issues surrounding tailpipe emissions and oil usage, see Section 1.2 (Samaras and Meisterling, 2008; Messagie, et al. 2010). This review has therefore focused on vehicles solely powered by batteries i.e. BEVs, however these still have many drawbacks. These include cost and range, which have been identified as the main obstacles to their uptake by consumers (Deloitte Development LLC, 2010).

The short ranges of BEVs result from the currently limited performance of batteries, which are addressed further in Section 2.3. However, the majority of trips are within the range of current BEV technologies (Matthe, et al. 2011). A potential solution to this problem is to incorporate a range extender unit e.g. a combustion engine, in conjunction with a battery pack sufficiently large to meet most trips (Matthe, et al. 2011; Varnhagen, et al. 2011; Ribau, et al. 2012). This would permit the vehicle to operate as a BEV for the majority of the time, while the additional energy unit would only operate on limited occasions. Range extenders will add mass, although potential exists to offset some of this through the use of smaller battery packs compared to conventional BEVs.

Batteries are also responsible for the majority of the higher costs of BEVs compared to conventional vehicles. Their costs are anticipated to drop substantially with mass production and technology refinements, but they will remain a large contributor to the overall vehicle. For example a 21kWh pack, in 2030, has been estimated to still cost around £3,500 (Offer, et al. 2010; Element Energy, 2012). The cost of conventional powertrains may increase in the future as they become more complex and require further equipment to meet tightening emissions standards, which could mitigate some of the difference (Element Energy, 2011).

The electricity source is a key aspect in determining the efficiency of BEVs, as discussed in the following section. However, there are many other potential areas for efficiency losses, see Figure 2.3 (Campanari, et al. 2009; Sato, et al. 2011; Defra, 2012). This shows that the efficiency gains of BEVs, resulting from the high efficiency of their motors compared to ICE, could be considerably eroded by combined downstream losses.

Feedstock extraction and transportation	x	Electricity generation	x	Electricity transmission	x	Vehicle charger/ battery	x	Vehicle motor and invertor	=	Overall efficiency
Natural gas 90		Natural gas 52		93		85		90	=	33%
Renewables 100		Renewables 100		93		85		90	=	71%

Values for percentage efficiencies and refer to a BEV charged using electricity produce from natural gas (top) and from renewables (bottom). The overall efficiency is the product of all the efficiencies.

Figure 2.3 Approximate well-to-wheels efficiencies of BEVs

Electricity generation and supply

The lifetime benefits of BEVs are highly dependent upon the impacts of the electricity used to charge them. The impacts of grid electricity vary considerably between locations, due to differences in grid mixes and efficiencies. This can lead to the effects of BEVs being location specific. For example, over 1.4kg of GHG emissions are associated with the production of one kWh of electricity using India''s grid, while Sweden''s grid emits only 0.05kg/kWh (Defra, 2012). This is due to India''s grid consisting mainly of coal power plants, while Sweden''s uses mainly hydro and nuclear.

An additional complication receiving attention in the literature is the impacts of marginal electricity (Thomas, C. E., 2009; Ma, et al. 2012). These are the impacts resulting directly from the additional electricity load that will be placed on a grid by BEVs. These impacts may be significantly different to those for the average grid, depending upon the source of the additional load. For example, Ma, et al. (2012) showed the well-to-wheels (which refers to the sum of the well-to-tank and tank-to-wheels phases) CO_{2e} emissions of a BEV increased by over 75%, when marginal electricity was used in place of average values. This results from the fact that the marginal electricity was assumed to be produced predominantly from coal, while the average value included renewables and nuclear used for base loads. However, marginal emissions could reduce substantially as the oldest, often highest emission plants, are replaced with more efficient alternatives (Hawkes, 2010). A further argument could be presented, that current marginal supplies are needed for current variable loads. Therefore, additional loads, e.g. large numbers of BEVs, would require the installation of additional capacity. New installations are likely to have below average emissions, lowering the values associated with BEVs. With restrictions on low emission energy sources e.g. cost, availability and practicality (see Section 1.2.1), it could again be argued whether vehicles are the optimal use. The same amount of low emission electricity could instead be first used to substitute other energy demands such as existing grid loads or heating oil. These options could offer greater overall benefits, depending upon their impacts compared to those mitigated by an electric vehicle, but this may overlook other gains such as reductions in urban pollution.

In contrast to the availability of other alternative fuels, electricity infrastructure is available in most populated areas. However safe charging points which are vehicle accessible will be required, along with potential network upgrades or additions, to meet increased demands (TfL, 2010). This will introduce additional costs e.g. the cost of installing a twin on-street charger is around £5000 to £7000 (Cenex, 2013). Existing domestic sockets can be used to charge BEVs, but owners are recommended to install dedicated supply units to improve safety (British Gas, 2013).

The time taken to charge BEVs also presents a further problem. For example, a current BEV, using a UK household supply, takes around 7 hours to charge. High power quick chargers could be used to reduce times to approximately 30 minutes for a 65% charge increase (Ikezoe, et al. 2012). This is still an order of magnitude higher than conventional vehicle fuelling times and the recharging efficiency can be reduced (Pollet, et al. 2012).

Options, such as battery swapping or dynamic charging, have been suggested to overcome these long durations but both have drawbacks. Battery exchange would require some standardisation of packs, investment to establish the infrastructure and incur safety issues due to the heavy packs and high currents involved (BERR and DfT, 2008). Dynamic inductive power transfer is being developed whereby power is transferred magnetically from coils mounted in roads to ones in vehicles (Qualcomm, 2013). To establish this system would require considerable investment in infrastructure and there may be a drop in efficiency, compared to good quality conductive chargers (Yilmaz, et al. 2012).

2.1.5. Summary of advanced powertrains and fuels

Substantial drawbacks were shown to be involved with all potential powertrains and fuels.

ICEs using conventional fuels cannot remain the staple of the fleet given their inability to meet long-term decarbonisation goals and fuel supply issues, although they may play an important part in short-term reductions.

Biofuels used in combustion engines could offer improvements. However, their production consumes significant amounts of energy and the problems associated with increased supply suggest that they will not be able to efficiently meet the majority of demands.

Hydrogen fuel cells can eliminate tailpipe emissions and oil dependency. Overall though the system is not energy efficient, due to the high energy consumption of hydrogen production, coupled with that incurred during storage, and losses in the fuel cells themselves. This is illustrated in Figure 2.4, where it can be seen that a vehicle using hydrogen produced from EU grid electricity has far higher well-to-wheels (WTW) energy consumption than a petrol vehicle. Even when using renewables, the total energy consumption is still around that of conventional vehicles. BEVs, however, can have far lower energy consumptions. This, along with their ability to eliminate tailpipe emissions, indicates they have the greatest potential to mitigate the problems of energy use and harmful emissions discussed in Chapter 1.



Figure 2.4 Vehicle well-to-wheels energy usage

The data presented in Figure 2.4 was calculated as follows:

- The New European Driving Cycle and parameters from a Mark 6 Volkswagen Golf were used to model the use phase, with manufacturer best in range data taken for the baseline vehicle consumptions.
- The hydrogen and hybrid vehicles were based on data from the Honda FCX Clarity and Toyota Prius hybrid respectively. Allowances were made for the differences between the size, coefficient of drag and frontal area of these vehicles and those of the baselines.
- Data for the BEVs was derived using a basic version of the MATLAB model described in Chapter 5.
- The tank-to-wheels energy consumptions for the remaining fuel types were assumed to be similar to those of the corresponding baseline vehicles, in line with the findings of JEC (2011a).
- The well-to-tank values were calculated using data from JEC (2011b) and Defra (2012). Hydrogen electrolysis was assumed to have an energy efficiency of 65% and 0.125MJ of electricity per MJ of hydrogen was included for compression (Armaroli and Balzani, 2011b).

2.2. Impact mitigation using non-powertrain vehicle parameters

The efficiency of a vehicle is not only determined by that of the powertrain it utilises, but also by other factors, such as mass and the coefficient of drag.

The following subsections review the main factors to establish their influence on vehicle efficiency, the feasible extent of their improvements and how they can affect comparisons between vehicle powertrains.

2.2.1. Light weighting

Mass is a serious problem for BEVs. Their battery packs typically add around 250 to 300kg to a "C"segment vehicle. This mass increases vehicle energy usage, which in turn necessitates a larger battery pack to accomplish a given range.

Vehicle light weighting can be achieved through design optimisation, the use of new materials or simply by vehicle downsizing. Innovative designs and alternative materials aimed at reducing mass are now featuring on production vehicles. For example, Jaguar have extensively utilised aluminium and magnesium in their models and BMW are planning a range featuring carbon fibre body shells (Jaguar, 2013; Kingston, 2013).

Literature values suggest materials substitution has the potential to reduce total vehicle mass by around 20% (Kasseris and Heywood, 2007; Lewis, et al. 2012). Mass reductions in one area can also enable secondary further benefits, whereby other components can be downsized due to lower loads (Lewis, et al. 2012). This leads to the benefits of mass reductions being magnified, but also to the problems of increased mass, being amplified.

Lightweight materials tend to have higher production impacts and costs than conventional steel. Figure 2.5 estimates the potential mass savings and CO_{2e} emissions associated with several materials when used to substitute a 1kg steel component (Coates, 2013; DOE, 2013; GaBi, 2013). The CO_{2e} emissions shown allow for the lower masses of the alternative materials needed, relative to steel, but still indicate a trend of increasing emissions with reducing mass. The figure refers to primary production, but the use of recycled materials can have a big impact. For example steel and aluminium are both readily recyclable, which will enable products with lower impacts. However recycling of carbon and glass fibres, is so far commercially limited, and thus so too are the potential benefits (Mayyas, et al. 2012).



Figure 2.5 Mass reductions and relative emissions of lightweight materials

2.2.2. Vehicle design

Equations (2.1) to (2.4) show how the total force required to propel a vehicle can be calculated.

Force (for a flat surface) =
$$F_{ad} + F_{rr} + F_a$$
 (2.1)

$$F_{ad} = 0.5 * \rho * A_v * C_d * V_e^2$$
(2.2)

$$F_{rr} = M * G * C_r \tag{2.3}$$

$$F_a = M * a \tag{2.4}$$

Where:

 F_{ad} = Aerodynamic drag force (N)

 F_{rr} = Rolling resistance force (N)

 F_a = Force required for acceleration (N)

 ρ = Density of air (kg/m³)

 $A_v =$ Frontal area of vehicle (m²)

 $C_d = Drag \text{ coefficient (dimensionless)}$

 $V_e = Velocity (m/s)$

M = Mass (kg)

 $G = Gravity (m/s^2)$

 C_r = Coefficient of rolling resistance (dimensionless)

 $a = Acceleration (m/s^2)$

The variables in equation (2.2) are frontal area, drag coefficient and velocity. Unless the vehicle can be made smaller or be driven at lower speeds, the frontal area and velocity are also reasonably set. This leaves the drag coefficient as the main area that can be addressed in vehicle design. Allowing for mass, discussed in Section 2.2.1, leaves the coefficient of rolling resistance as the variable in equation (2.3) and acceleration in equation (2.4). Similar to velocity, within limits, the acceleration is controlled by the vehicle's use.

The drag coefficient is a function of a vehicle"s shape. Values have been steadily decreasing from around 0.4 in 1980, to 0.25 for some recent optimised vehicles, such as the Toyota Prius and Audi A2 (Hucho, 1998). Optimum practical streamlining is suggested to result in a figure around 0.15 to 0.2. Further reductions are possible, but require bodies with impractically large length to height ratios, i.e. vehicles would need to be very long to allow sufficient height for the occupants (Hucho, 1998; Bosch, 2004). Future reductions are therefore anticipated, but the magnitudes of the improvements are likely to decrease into the future as designs approach practical limits.

Rolling resistance mainly results from deformation of the tyres as they pass over the road surface. The road itself also contributes, with rougher surfaces increasing the value (Bosch, 2004; Wang, et al. 2012a). The rolling resistance of tyres has been decreasing by approximately 1% per year and good values are now around 0.007 (Fontaras and Dilara, 2012).

2.2.3. Potential issues in assessments

Improvements to the factors described above, e.g. mass and the coefficient of drag, can be used to improve a vehicle regardless of the powertrain it uses. Vehicles with alternative powertrains, which are designed to provide optimum efficiency, typically have these non-powertrain parameters far more optimised than conventional vehicles. For example, the energy required to propel a vehicle with a coefficient of drag and frontal area, equal to the 2010 Toyota Prius over the New European Driving Cycle (NEDC), is approximately 8%

lower than for one modelled using the parameters for a MK6 Volkswagen Golf of the same year. This assumes no powertrain losses, a mass of 1300kg and all other parameters are identical.

This creates problems in many comparisons based on different vehicles, even if they are of similar sizes or classes. Many comparisons also provide limited data on these parameters, making their consistency uncertain (Messagie, et al. 2010; Notter, et al. 2010; Torchio and Santarelli, 2010). When reviewing the results it is often not possible to distinguish what benefits are due to the powertrain and what result from the other parameters. Often all appeared to be attributed to the alternative powertrain. This can lead to overestimations of the benefits of the powertrain itself.

2.3. Battery technologies

2.3.1. Background

The specific energy of batteries is currently around 100 times lower than that of petrol. This creates a major barrier to BEV uptake, because it is insufficient to enable their ranges to approach those we have come to expect from modern ICE vehicles. Increasing the mass of batteries can help improve the range but this will compromise space, add further cost and increase the vehicle's energy consumption, which results in decreasing range improvements for larger batteries.

To avoid the mass, cost and efficiency of BEVs being overly compromised, mainstream manufacturers appear to be keeping the battery pack mass below 300kg (IDIS, 2011). Using this as a maximum mass and a BEV energy consumption of 0.2kWh/km (Campanari, et al. 2009), would require a battery capable of producing >330Wh/kg to achieve a range comparable to a basic ICE vehicle of 500km. If the battery depth of discharge (DOD) was limited to 80%, to improve life (Element Energy, 2012), this would increase to >410Wh/kg. This value is at the pack level and additional components, e.g. cabling and cases, mean the cell specific energy would need to be yet higher (Matthe, et al. 2011). From Table 2.2, it can be seen that this is several times greater than that offered by current batteries.

Battery type	Specific Energy	Specific Power	Number of cycles	Energy
	(Wh/kg)	(W/kg)	down to 20% SOC	efficiency %
Lead-acid	35-50	150-400	1000	70-84
Nickel cadmium	50-60	80-150	1000	65-85
Nickel-metal hydride	70-95	200-300	1200+	65-85
Lithium-ion	80-180	200+	1000+	>85

(Ehsani, et al. 2010; Rydh and Sanden, 2005; Ikezoe, et al. 2012; Pollet, et al. 2012; Goodwolfe Energy, 2013)

Table 2.2 Average performances of various battery technologies

It is not only the specific energy that will affect the suitability of a battery for use in a BEV. Other vital parameters include:

- Specific power. The battery will need to supply sufficient power to meet propulsion and auxiliary demands, even at low states of charge (SOC). For a "C"segment sized BEV, a power output of around 100kW is necessitated (Ikezoe, et al. 2012). This would require a specific power of over 330W/kg (at the pack level), for a 300kg battery pack. Cells however are designed differently to achieve high specific powers, compared to high specific energies, which introduces trade-offs between these parameters.
- Energy efficiency, ratio of energy input to energy output. This impacts the overall energy requirements of the vehicle.
- Lifetime. Will a battery pack need replacing during the vehicles life?
- Permissible DOD. To help improve lifetimes, avoid overcharge situations and ensure power demands can be met (maximum power decreases with SOC), the battery may not be fully charged or discharged. For lithium-ion BEV packs, typically only 80% of the capacity is used (Element Energy, 2012).
- Cost.
- Safety.

Average values for some of these factors are shown in Table 2.2. Lithium-ion stands out from the other battery types, because it can meet the power requirements, has a relatively

high energy and offers good efficiency. Compared to lead acid though, it is more expensive and requires additional safety measures.

Due to these considerations lithium-ion batteries are the current choice for many BEVs. They are also expected to remain so in the coming years, in view of the challenges facing the deployment of advanced batteries, discussed in Section 2.3.3 and due to past development rates indicating that it may take a decade or longer for new technologies to be deployed in vehicles (Element Energy, 2012). Subsequently, lithium-ion batteries were chosen as the basis of the LCA developed in Chapter 4.

The following sections review the characteristics of lithium-ion batteries and provide a brief review of the potential of new chemistries to mitigate the issues discussed above.

2.3.2. Lithium-ion

Lithium-ion batteries store and relinquish energy through the movement of lithium ions between the cathode and anode. The electrolyte does not form part of the chemical reaction and mainly serves as a medium to permit the effective transmission of ions, while preventing the flow of electrons. Equations (2.5) and (2.6) show the reactions at the cathode and anode, respectively, for a lithium-cobalt-oxide variant (LiCoO₂). The discharge reaction is read left to right and charge right to left.

$$Li_{(l-x)}CoO_2 + xLi^+ + xe^- \leftrightarrow LiCoO_2$$

$$(2.5)$$

$$C_6 Li_x \leftrightarrow 6C + xLi^+ + xe^- \tag{2.6}$$

Many different variants are in production, which are often distinguished by their cathode material. The most common are outlined in Table 2.3. This shows that each has their own advantages and disadvantages, which may result in different optimal choices depending upon the intended application.

Currently LMO materials are commonly used for BEVs. However, LFP is being used due to the improved safety and cycle lives it offers, and NCM to increase capacities (Lowe, et al. 2010; Matthe, et al. 2011; Dow Kokam, 2013).

Along with the cathode, other cell constituents can also vary. For example graphite is extensively used as the anode material, but other options exist, such as lithium titanate oxide which offers improved cycle lives, but lower specific energies and higher costs (Burke and Miller, 2009).

Cathode	Specific	Specific	Life	Cost	Safety
	energy Wh/kg	power			
Lithium cobalt oxide	170 to 185	Medium	Low	High	Poor
(LCO)					
Lithium iron phosphate	100 to 140	Good	Good	Low	Good
(LFP)					
Lithium manganese	90 to 150	Good	Low/	Low	Medium
oxide (LMO)			Medium		
Lithium nickel cobalt	155 to 185	Medium	Medium	Medium	Medium
manganese (NCM)					

(Matthe, et al. 2011; Element Energy, 2012; Väyrynen and Salminen, 2012)

Table 2.3 Properties of common lithium-ion battery chemistries

Three key considerations that have been incorporated into the LCA performed in Chapters 4 and 5 are battery lifetime, energy efficiency and recycling. These factors have therefore been further discussed below, along with a brief overview of the potential hazards of lithium-ion batteries. Production is also an important aspect in this thesis, but is discussed later in the inventory for the LCA.

Safety

Safety is a major concern for lithium-ion battery packs. Abuse or damage e.g. overcharging or short circuit, can cause them to go into "thermal runaway" (Balakrishnan, et al. 2006). This is where elevated temperatures cause exothermic reactions between the electrodes and the electrolyte. These in turn further increase the temperature, causing additional materials to react and can result in explosions and fires (Baginska, et al. 2012).

To help prevent dangerous or detrimental situations, safety features such as shutdown separators, vents, and reaction reducing coatings are used. In large lithium-ion packs a battery management system (BMS) is also necessitated. This monitors parameters, such as the temperature, current and cell voltage, and should isolate the pack or cells if out of range values are detected (Doerffel, 2007).

Lifetime

A variety of processes, occurring during both storage and use, cause the capacity and power of lithium-ion cells to decrease. For example, the solid electrolyte interphase initially created during the formation cycle will continue to propagate, reducing the capacity and increasing the impedance (Vettera, et al. 2005; Sankarasubramanian and Krishnamurthy, 2012).

Use conditions such as DOD, temperature and charge/discharge rates can alter lifetimes considerably. Therefore the actual lifetime of a vehicle battery pack will depend upon how, and where, the vehicle is operated. For example, storage at high temperatures and states of charge accelerate aging, while low temperatures can lead to lithium metal plating which also results in aging and safety issues (Vettera, et al. 2005). Figure 2.6 shows the effects of variations in storage temperature on the capacity of a NCM cell (Käbitz, et al. 2013). This indicates that battery packs utilised in hot climates could have far shorter life expectances.

The processes involved, their interactions, various in-use conditions and manufacturing differences, make lifetime predictions extremely complex (Vettera, et al. 2005; Sankarasubramanian and Krishnamurthy, 2012). These considerations, coupled with limited long term aging tests (Käbitz, et al. 2013), and numerous different types of lithium-ion batteries, mean predictions could vary significantly. However, LFP cells are generally quoted as having the highest cycle lives of the common chemistries (incorporating graphite anodes), with values of over 2000 cycles to 80% DOD often reported (Peterson, et al. 2010; Väyrynen and Salminen, 2012; Mulder, et al. 2013).



(Constructed using data from Käbitz, et al. (2013))

Figure 2.6 Effects of temperature on cell capacity degradation

Energy efficiency

The energy efficiency of lithium-ion batteries deteriorates as they age. Data is limited in the existing literature, but results from one set of long term tests showed an initial energy efficiency of 94%, which dropped in an approximately linier fashion to 91% after 400 cycles. The deterioration then appeared to accelerate slightly, dropping to about 84% after 800 cycles (Kuhn, et al. 2005).

Considering the lifetime of BEV battery packs, this effect could have a significant impact on the overall vehicle. The above figures demonstrate that after 800 cycles nearly 12% more energy would be required, compared to when the battery pack was new.

Estimations of energy efficiency are further complicated by variations with the batteries SOC, charge/discharge rates and temperature. Lower temperatures, and higher charge/discharge rates, tend to reduce the efficiency (Kuhn, et al. 2005; Burke and Miller, 2011; Mulder, et al. 2013). For example, simulations by Smith and Wang (2006) showed the efficiency of a vehicle battery pack dropped by about 2% as the temperature decreased from 30°C to -15°C. Further results, for tests on a variety of LFP cells, showed an average decline in efficiency of approximately 8% when the discharge rate was increased from 1C to 5C (Mulder, et al. 2013).

The materials and processes used to manufacture cells introduce yet more potential variation. Tests have shown trends between cathode chemistries, which could be an important consideration in battery selection for BEVs. NCM cells were found to generally have higher efficiencies, with values around 94% (for a 1C discharge rate), compared to around 90% for LFP cells (Omar, et al. 2012; Mulder, et al. 2013).

Recycling

End-of-life (EoL) treatment of vehicles and batteries is necessitated to meet regulations and will have an impact on their LCA results. It must therefore be considered when evaluating BEVs. In the EU Battery Directive (Council Directive 2006/66/EC), a minimum recycling target of 50% by mass for lithium-ion batteries is stipulated.

Two different techniques are currently used for the recycling of lithium-ion cells (Georgi-Maschler, et al. 2012). The first is a pyrometallurgical process where high temperatures are used to separate the valuable metallic fractions. The second is a hydrometallurgical process where metals are separated via liquid processes, such as leaching and precipitation,

following mechanical shredding of the cells. These descriptions indicate the main processes involved, however numerous variations and combinations of these methods have been proposed (Xu, et al. 2008; Georgi-Maschler, et al. 2012).

The pyrometallurgical process is indicated to have a recycling efficiency of greater than 50% in terms of mass, which is needed to meet EU targets (Umicore, 2012). The high temperatures in this process result in the plastic and carbon content of the cells, either acting as reducing agents, or being incinerated as fuel. However, only that used as a reducing agent counts towards recycling targets (Commission Regulation (EU) No 493/2012). The process also only recovers certain metals (Co, Ni, Cu and Fe), while the lithium, manganese and aluminium fractions are lost in slag (Umicore, 2012). Most cells currently being processed are from consumer electronics and contain cobalt in their cathodes and steel in their cases. These are both recycled and represent a significant proportion of the mass (Fisher, et al. 2006). This is not the case for many electric vehicle (EV) cells, which utilise different materials and may result in the pyrometallurgical process not offering sufficiently high recycling rates to meet targets.

Hydrometallurgical processes offer the potential to recoup more materials and are suggested to have lower energy requirements (Fisher, et al. 2006). This option has therefore been used in the subsequent LCA in Chapter 4 and further process details are provided therein.

There are also other major considerations concerning recycling, such as will the pack need to be dismantled (which can be very time consuming and costly), where the batteries are to be processed (e.g. will only a few processing plants be feasible, necessitating long distance transportation) and whether re-use is an option. Figure 2.7 shows some of these options along with simplified flows for the two main recycling routes.



Figure 2.7 Potential recycling routes

The actual end-of-life processes used will also be dependent upon the aims and their relative importance, see Figure 2.7. For example, these could be:

- To maximise the revenue.
- To maximise the recycled fraction. Minimum recycling fractions are dictated by legislation.
- To reclaim scarce or specific grades of materials. For example, materials may only be sufficiently purified for effective sale or to be classed as recycled, rather than for re-use in new batteries.
- To minimise factors such as emissions, energy consumption and landfill.

Ideally, optimisation of all these aims would go hand in hand to form a hypothetical "ideal" scenario. To some extent this will be possible, e.g. increasing the recycled fraction will produce more valuable materials which will increase revenues. However, particularly when going to the extremes in any of the factors, the benefits may be more than offset by reductions in others. For example recycling a fraction of the battery may be achieved at a reasonable price, but higher rates may result in costs and energy consumptions which exceed those recouped by the additional materials reclaimed.

Cost could be a significant barrier to lithium-ion battery recycling. Existing processes currently target the valuable nickel and cobalt fractions, with other materials such as lithium and manganese often not being recovered (Dewulf, et al. 2010; Umicore, 2012). Most lithium-ion batteries currently being processed are LCO versions, which contain significant amounts of cobalt (Lowe, et al. 2010). For cost and safety reasons, variants with different cathode materials e.g. LMO and LFP, whose materials have little value, are being used in BEVs.

Presently, although required by legislation, the vehicle recycling industry in the EU works on the basis that vehicle reclamation is profitable (Savage, et al. 2010). It is presently unclear as to how BEVs will affect this, given the considerations above. However, other components in the pack e.g. the casing and the wiring, and the vehicles as a whole, are likely to have a value at end-of-life.

2.3.3. Alternative chemistries

Improvements in the specific energy of lithium-ion batteries are anticipated, but they will be insufficient to enable practical BEVs with ranges approaching those of ICE vehicles. Several alternative batteries, chiefly metal-air and lithium-sulphur, are being investigated which could offer much higher energies (Peled, et al. 2011; Thackeray, et al. 2012; Zhang, 2013). The potential for improvement is indicated by the theoretical specific energies of these batteries, some of which are given in Table 2.4. For example, the value for lithium-air is nine times that of lithium-ion. Further details on the operation and problems associated with these are given in the following subsections.

The theoretical specific energy of a battery is a function of the molecular mass of the materials involved (M_i), the number of electrons transferred (n_e) and the voltage generated (V), see equation (2.7) (Ehsani, et al. 2010).

Theoretical specific energy
$$(Wh/kg) = [96495*n_e*V] / [3.6* \sum M_i]$$
 (2.7)

Battery	Theoretical specific energy (Wh/kg)
Li-ion (value for LCO)	390
Zinc-air	1090
Lithium-sulphur	2570
Lithium-air (including O_2 and taking Li_2O_2	3500 (5200 sometimes quoted if Li_2O can
as product)	be attained as the product)

(Adapted from Bruce, at al. 2011)

Table 2.4 Advanced battery performances

The relationship in equation (2.7) suggests materials such as lithium, sodium, oxygen and sulphur would make superior material choices, due to their low masses and high electropositivity/electronegativity (Ehsani, et al. 2010). Unfortunately the specific energy feasibly available from a battery is well below the theoretical value, typically <1/3. This results from, the additional masses introduced by the battery case, terminals and electrolyte solvents for example, that do not form part of the reactants and various restrictions that act to lower the cell voltage (Ehsani, et al. 2010; Bruce, at al. 2011). Practical values will therefore be substantially below those shown in Table 2.4.

Metal-air batteries

Metal air batteries consist of a porous cathode, typically carbon with a catalyst, an electrolyte, and a consumable anode, e.g. aluminium, zinc or lithium. During operation oxygen is absorbed through the cathode and reacts with metal from the anode to produce a current. The rest of this section has focused on lithium-air variants, due to their high energies, however many of the problems mentioned are applicable to other air-batteries.

Due to the considerations given in the previous section, the attainable specific energy of lithium-air batteries is expected to be less than 1000Wh/kg. This should still be sufficient for long range EVs, >500km (Bruce, at al. 2011). However, there are several major obstacles that need to be overcome before they can be practically used in vehicles. Some of these are:

- The formation of lithium dendrite during charging, which can result in poor cyclic performance, internal short circuiting and safety issues.
- The discharge products are insulating, which necessitates a large surface area for the reactions to occur over.

- Oxygen from the air can be used to feed the cell, but other gases present e.g. CO₂ and water, can affect their operation. Therefore these need to be removed, while still allowing fast O₂ diffusion.
- Insufficient cycle life, usually less than 100 cycles.
- Low energy efficiencies, currently around 60 to 70%.
- The safety issues raised by using metallic lithium, e.g. violent reactions with water.
- Low powers (Peled, et al. 2011; Wang, et al. 2013).

Lithium-sulphur

The construction of lithium-sulphur batteries is similar to that for metal-air batteries, with the main differences being that their cathodes contain sulphur particles and do not adsorb oxygen. On discharge lithium ions from the anode combine with the sulphur, ultimately forming lithium sulphide.

The problems are also similar to those given in the previous section for lithium-air batteries. However, contamination from the air is not a problem, but capacity fade and high self-discharge rates are, due to the formation of soluble alternative lithium sulphur compounds (Bruce, at al. 2011; Zhang, 2013).

2.4. Summary

This Chapter provided an appreciation of the main powertrains and fuels proposed to help address the problems associated with current road vehicles. It also identified and discussed several factors that have commonly introduced irregularities into assessments of their impacts. These findings helped, focus the subsequent research and ensure that existing problems were either mitigated or studied. The key findings of the Chapter are outlined below.

Out of the currently proposed alternative powertrains and fuels, BEVs were identified as having the greatest potential to mitigate the energy and emissions impacts associated with conventional vehicles.

Improvements in non-powertrain factors, such as the coefficients of rolling resistance and drag, where shown to help mitigate vehicle impacts regardless of the powertrain. However, in many existing comparisons, inconsistencies and a lack of documentation on these factors can result in misinterpretations of the benefits resulting solely from an alternative powertrain choice.

Mass is an important consideration affecting vehicle energy usage, particularly for BEVs, where it places practical limits on their battery pack size. Lightweight materials could be used to reduce a vehicle"s mass and therefore, in-use energy, but the mass reductions they offer were generally found to be inversely proportional to their production impacts. Care is thus needed to ensure that increases in the production phase do not out way any in-use benefits.

The approximate battery performances needed, to enable BEVs with ranges similar to basic ICE vehicles, highlighted the extent of the improvements required over current chemistries. Future chemistries were identified which could enable long ranges, although all were found to have major problems that are expected to take many years to resolve, before they can be practically used in vehicles.

Lithium-ion batteries were identified as the most likely choice for BEVs now and in the coming years. Significant variation was found within the range of lithium-ion chemistries, not just in terms of their specific energies, but also in their lifetimes and energy efficiencies. These parameters could have major influences on the impacts of BEVs and need to be included in LCAs to ensure optimal choices are identified. Many LCAs of electric vehicles assume a single generic lithium-ion battery, which can lead to discrepancies compared to those used in actual vehicles.

3. REVIEW OF EXISTING LIFE CYCLE ASSESSMENTS

3.1. Introduction

There are many phases involved in the lifetime of a vehicle. The flow chart in Figure 3.1 highlights the energy, emissions and material flows associated with the mains phases.

Due to the variety of options available for the production and supply of a vehicle"s in-use energy source, commonly called the well-to-tank (WTT) phase, these were covered separately in Figure 3.2. This shows the processes required to produce several vehicle fuels using three different primary energy sources, fossil fuels, crop feedstocks (i.e. biofuels) and nuclear/renewables (e.g. wind and solar but excluding biofuels). Each flow path represents a potential fuel supply route, indicating the multitude of different production options and the green arrows signify transfers between phases, which usually incur further energy use and emissions on top of those for the processes themselves. Further details on some of these fuels (e.g. hydrogen and electricity) were given in Chapter 2.

Life cycle assessment (LCA) is a methodology used to assess the environmental aspects of a product"s lifetime. The method aims to encapsulate all significant environmental impacts, from raw materials extraction to end-of-life, in order to quantify the whole life performance of a product. The purpose is to provide recommendations on where, in a product"s lifetime, impacts require abatement and to help identify optimal choices (British Standards Institution, 2006a).

Automotive manufacturers are increasingly using LCA to assess and minimise the detrimental effects of their vehicle production, use and disposal. Many manufacturers, including, Ford Motor Company, Volkswagen and Volvo, have been performing LCAs since the 1990's and are now increasingly integrating the methodology into their initial vehicle design phases. These early considerations help, maximise the attainable improvements and minimize the associated costs, because less rework is required (Chanaron, 2007).

LCA is also a powerful tool for assessing the potential of new powertrains. The past decade has seen a number of such assessments being produced, which compare their environmental burdens to those of conventional powertrains, e.g. Samaras and Meisterling (2008), Ma, et al. (2012) and Hawkins, et al. (2013).



Figure 3.1 Processes involved in the lifecycle of a vehicle



Figure 3.2 Process routes for the provision of a vehicle's in-use energy

However, many assessments have confined themselves to the well-to-wheels (WTW) phases (Kasseris and Heywood, 2007; Campanari, et al. 2009; Torchio and Santarelli, 2010). This is due to the complexity and cost of a full LCA, which encapsulates all relevant aspects, and previous findings which suggest the WTW phases consume over 80% of a conventional vehicle's lifetime energy (Torchio and Santarelli, 2010). This may not be the case for alternative powertrains, where higher production impacts, coupled with lower WTW values, lead to the other phases (see Figure 3.1) becoming far more significant in a vehicle's lifetime.

The concentration on the WTW phases has led to a respective shortfall in data regarding the production and disposal impacts of alternative powertrain components. This is a particular problem for electric vehicle batteries, due to their potentially large impacts and the extensive variation reported in the few existing studies (Dunn, et al. 2012a).

Therefore to improve evaluations of whole life BEV impacts, an improved LCA of their production is needed. Many of the components used by BEVs are often similar to those of

conventional vehicles (e.g. the body shell and interior). This should allow them to be modelled reasonably accurately using LCA data from conventional vehicle production. However, other components primarily their batteries, motors, power electronics and wiring, will introduce discrepancies. Out of these, the batteries are the largest contributor to the production impacts (Notter, et al. 2010), and were subsequently chosen as the main focus for the LCA developed later in this thesis.

This Chapter first provides an overview of the main LCA standards and methodologies used, looking at their individual differences and merits. This is followed by a brief review of existing research which has quantified and compared the impacts of alternative powertrains. The review then focuses on LCAs that have specifically addressed the production and recycling of lithium-ion vehicle batteries. Finally, additional battery parameters which can influence whole life electric vehicle assessments are quantified and the key chapter findings summarised.

3.2. Life cycle assessment

Several standards are available which describe the procedures and contents of LCAs. These help to guide practitioners and improve consistency and transparency in assessments. The most relevant LCA standards and methodologies are outlined below.

3.2.1. Standards

European Standard EN ISO 14040:2006

ISO 14040 (British Standards Institution, 2006a), lays down the basic framework for conducting an LCA, and is supplemented by further details provided in ISO 14044 (British Standards Institution, 2006b). The standard defines an LCA as a full cradle-to-grave analysis of a product"s life cycle, encapsulating initial materials extraction through to recycling/disposal and segregates the assessment into four key parts:

- Definition of the goals and scope. The goals should establish why the analysis is to be performed while the scope should include, for example, definition of the functional unit, the factors that are assessed, the assumptions used and the analysis boundaries.
- 2. Inventory analysis. This is where data on the inputs and outputs required to assess the defined factors are gathered, e.g. materials and energy used.

- 3. Impact assessment. This phase establishes the importance of the factors assessed, in terms of environmental impacts, by associating the inventory data with relevant impact categories. The additional results provided are intended to help decision making in the following stage. In studies where the results of the Inventory analysis provide sufficient information, this phase may be superfluous.
- 4. Interpretation. This section should make recommendations in line with the defined assessment goals and contemplate the limitations of the study.

The standard also highlights several other aspects that are important in conducting a comprehensive LCA:

- Transparency. This is necessary to ensure the results of an LCA can be correctly interpreted and fairly compared with other assessments.
- Comprehensiveness. Ideally all environmental, resource and health aspects would be included. However, due to financial, time and data availability issues, the scope of LCAs have to be restricted, usually to the aspects which are suspected as having the most significant influences.
- Iteration. Data from each phase should be iterated between phases to aid accuracy, e.g. if a process or emission is found to have higher than anticipated impacts, the scope and inventory could be expanded to encompass a more detailed analysis of this factor.

To try and establish how products or processes compare, many LCAs use weighting factors, to amalgamate all the impacts into a single term. However, weighting can lead to inconsistencies between comparisons, depending upon the chosen weighting factors and ISO 14040 states that (British Standards Institution, 2006a, p9):

,there is no scientific basis for reducing LCA results to a single overall score or number, since weighting requires value choices^{**}.

Due to the variety of tasks and industries, that LCA can be applied to, the Standard allows great flexibility and acknowledges that there is no single method. This means that there may be discrepancies between LCAs performed on the same or similar products, even if they are compliant with the Standard. This may make it difficult to compare and contrast their results accurately (European Commission JRC, 2010).
Further guidelines

The ISO 14040 series is extensively used within the field and the basic methodology has been employed in the LCA performed in this thesis. However, there are several other guidance documents that build on the ISO 14040 series surrounding LCA and sustainability (Finnveden, et al. 2009). These include:

- PAS (Publicly Available Specification) 2050:2011, "Specification for the assessment of the life cycle greenhouse gas emissions of goods and services" (British Standards Institution, 2011a). This builds on the ISO 14040 series by providing more specific information for assessing GHG, with the aim of facilitating the production of clear and consistent assessments.
- BS 8905:2011 ,,Framework for the assessment of the sustainable use of materials Guidance". This standard addresses materials consumption by proposing an expanded general framework, which encompasses social and economic considerations, along with environmental aspects to help facilitate more sustainable materials usage (British Standards Institution, 2011b).
- The International Reference Life Cycle Data System (ILCD) (European Commission JRC, 2010). This consists of a substantial series of technical documents which provide additional guidance to the ISO 14040 series to help ensure consistency and quality in LCAs.

3.2.2. Life cycle assessment methodologies

Several different LCA methodologies have been developed, which can also influence the results of assessments. The most significant in the current literature are consequential, attributional and input-output-LCAs, which are summarised below (Matthews and Small, 2000; Thomassen, et al. 2008).

Consequential and attributional methodologies

The differences between consequential and attributional LCA methodologies, and how these can influence the results of LCAs, have received significant attention in the recent literature (Thomassen, et al. 2008; Brander, et al. 2009; Finnveden, et al. 2009). The key differences between the two methodologies are:

• Attributional LCA focuses on the emissions and material flows from a product or process and aims to quantify the total life cycle figures that directly relate to this.

• Consequential LCA aims to quantify how environmental factors will change in response to an alteration in demand, for example those resulting from a policy which encourages the use of a new product.

Consequential LCAs can be advantageous to help establish the impacts of systems into the future. However, predictions of how systems may respond to future demand changes and how these may influence their impacts, usually involve a large degree of uncertainty and complexity (Finnveden, et al. 2009). For example, increased demand for a material could lead to lower grade reserves being exploited, which may incur higher impacts, or it may lead to investment in new extraction, processing or recycling technologies, which could lower impacts.

Input-Output life cycle assessments

Unlike process based methodologies, where the inputs and outputs for each material and process are quantified and summed, an input-output LCA calculates values based on relationships between industry sectors.

Input-output analysis was derived as a method to explain how economic activities in one sector influence those in others (Leontief, 1970). However, the method has been extended to incorporate other issues, such as environmental impacts, which results in what is commonly referred to as an input-output LCA.

The methodology uses matrix theory to calculate upstream flows. This overcomes the problem of having to impose cut-off criteria when dealing with systems that interact with one another (further details on the theory can be found for example in Leontief, (1970)).

Input data is based on average data for industrial sectors, which can reduce the work associated with gathering inventory data. This allows assessments to be performed quicker and at a lower cost than process based LCAs. However, because specific processes are not modelled, the accuracy of results can be poor, depending upon how far the factor being assessed deviates from the sector averages contained in the input-output model. The databases also tend to be based on existing economic models. This means they are reliant on the accuracy of these and there being a sufficient relationship between the economic activity of a sector and the resulting environmental impacts (Matthews and Small, 2000; Hendrickson, et al. 2006). This has led to input-output LCAs not being viewed as a suitable alternative to process based assessments. However, they could be used to supplement

models, by helping to provide estimates for missing upstream data (Finnveden, et al. 2009).

3.3. Existing vehicle life cycle assessments

This section briefly reviews some of the vehicle production LCAs, which provide the most detail on their underlying data and methodologies, and looks at some of the reasons for variations. Due to the importance of batteries in this thesis, works which have focused on battery LCAs were reviewed more extensively in the following section.

3.3.1. Life cycle assessments of alternative powertrains

The GREET (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) Transportation Vehicle-Cycle Model developed by Argonne National Laboratory is a substantial Excel based assessment tool (Burnham, et al. 2006; Wang, et al. 2012b). It adds to their earlier fuel cycle model (which analysed the WTW aspects of fuel sources), to facilitate evaluations of the energy and emissions resulting from vehicle production, use and disposal. The model permits assessments of several powertrains, using both conventional and lightweight materials.

Transparency is an advantage of this model because flows can be traced within the Excel database back to base materials and an accompanying document provides additional information on the input data. The model calculates the impacts by adding fixed values for assembly, painting and recycling to those resulting from the production of the materials consumed in a vehicle (Burnham, et al. 2006).

Table 3.1 give some of the merits, limitations and assumptions identified for the GREET model. These suggested the model could be very useful for making base evaluations of vehicles without the need for expensive software or databases. However, the production data only encompasses a relatively limited number of materials, which means some impacts are excluded from the results, and it is mainly confined to US scenarios. Additional materials and processes could be incorporated, but would require significant work to expand and modify the already substantial Excel spreadsheets. This highlights that to practically build a model which encompasses more materials and processes, while maintaining ease of use and meeting timeframes, requires not only a large inventory database (such as those offered by GaBi and Ecoinvent), but also a specialist interface (e.g. GaBi and SimaPro).

Merits	Limitations and assumptions
The model was parameterised and	Only a limited number of materials were
permitted users to input some of their	modelled. Some materials, about 2% of the
own data or make predefined selections.	vehicle mass, were therefore not included.
Freely available.	Transportation of materials between
	processes is excluded.
Input data could be located in the	Some of the materials modelled were
spreadsheets which allowed the figures to	approximated using data for others. For
be interrogated and verified.	example cobalt and lithium oxide were
	based on data for nickel.
Several of the emissions were segregated	Vehicle assembly was based on one fixed
to approximate how much occurs in	value. This approach simplified the analysis
urban environments, where they have the	but provided limited detail on the scope and
greatest effect on human health.	may not be indicative of alternative vehicle
	assembly.

Table 3.1 Merits and limitations of the GREET model

WorldAutoSteel has developed a separate Excel model, for the purpose of assessing the effects of materials substitution (Geyer, 2012). The production phase mainly confines itself to processes and materials that are estimated to be substantially altered during materials substitution, although a value for battery production (taken from another assessment) is included.

Two major further works that have conducted LCAs of BEV production are Notter, et al. (2010) and Hawkins, et al. (2013). Notter, et al. (2010) focused on battery production and showed BEVs could offer clear reductions in environmental burdens over their whole life, compared to a petrol ICE vehicle. The inclusion of a comparison efficient diesel vehicle could however reduce the differences in some categories and the battery production impacts are possibly underestimated compared to other assessments, see Section 3.4.

The report by Hawkins, et al. (2013) modelled the influences of two different lithium-ion batteries, nickel cobalt manganese (NCM) and lithium iron phosphate (LFP), on the whole vehicle life using the battery LCA given in Majeau-Bettez, et al. (2011), see Section 3.4. However, they only assessed the direct differences in the battery production impacts and did not include the other effects of lifetime and efficiency also discussed in Majeau-Bettez, et al. (2011).

Compared to conventional vehicles, Hawkins, et al. (2013) showed BEVs can offer GHG reductions, but that they are subject to the electricity source and that different results may be obtained for other impact categories. The majority of some impact categories, e.g. human toxicity and mineral resource depletion, were shown to result from the vehicle and battery production, with the additional copper and aluminium content of BEVs stated to be major contributors to many categories.

A review of their input materials revealed that the BEVs were assumed to contain inverters for the motor and charger, each weighing 74kg. These components added 71kg of copper and 69kg of aluminium, with a further 60kg of aluminium suggested for the BEV cooling system. These requirements were in addition to those in the batteries, motor and base vehicle. The masses of actual suitable motor control units and chargers (inverters) were found to be much less, e.g. 16.2kg for the Nissan Leaf inverter assembly (Burress, 2012). The assumed aluminium and copper content of the BEVs are therefore expected to have been severely overestimated, which will in turn have substantially impacted on their final conclusions.

Several other vehicle production LCAs have been published, including many from manufacturers such as Volkswagen and Daimler (Volkswagen AG., 2008; Daimler AG, 2012). However, they mainly only cover conventional vehicles and most only present the results of their assessments, which precluded suitable review of their methodologies.

These assessments indicate that the overall impacts for conventional vehicles are decreasing with newer models. Most of this is resulting from the WTW phase, due to improvements in fuel economy, while the production phase impacts appear to be fairly constant (Volkswagen AG., 2008; Daimler AG, 2012). This is resulting in a relative increase in the importance of the production phase, in the whole vehicle lifetime, even for conventional ICE vehicles.

Variations in comparison vehicles and test cycles

The results of assessments which compare powertrains are very subjective to the chosen vehicles. When drawing comparisons discrepancies can arise from differences in the non-powertrain factors (see Section 2.2.3), and variations in the technology level. The high rate of fuel efficiency improvements for ICE vehicles seen in recent years (Daimler AG, 2012; SMMT, 2013), mean assessments not only need to encompass what vehicles are being

assessed, but also when. For example are the vehicles assessed representative of current fleet averages, state of the art technology or potential future advancements.

The potential extent of the effects arising from these factors can be highlighted using existing assessments, such as Hawkins, et al. (2013). In this assessment the use phase requirements, for ICE and electric vehicles, are based on values for the Mercedes A Class and Nissan Leaf respectively. These were suggested to be comparable due to their similar size, mass and power. The fuel efficiency for their baseline ICE vehicles is approximately based on average values for the vehicle range. However, the best-in-class figures for the new 2012 Mercedes A Class, 5.5 litres/100km for the petrol and 3.8 litres/100km for the diesel (Mercedes-Benz, 2012), are 20% and 30% lower respectively. These models were on sale alongside the BEV (Nissan Leaf) used in the analysis and indicate that if the assessment were repeated using these updated values differences in some of the final results would be obtained.

Many assessments model the use phase over standard test cycles, such as the New European Driving Cycle (NEDC). This has the advantage of allowing assessments to be more easily verified and compared. However, different values are likely to be obtained during real-world usage. For example, the NEDC is often seen to underestimate the actual in-use requirements, with average discrepancies of over 20% suggested (Samuel, et al. 2005; Transport and Environment, 2013). This will not only lead to low results, but also to variations in how the whole life impacts appear to be split amongst the phases.

The assumed vehicle lifetime distance is a further common source of variation in assessments. This again affects the total results as well as the split between production/end-of-life (EoL) and use impacts, due to the manufacturing/EoL impacts being averaged over different values.

3.4. Existing battery life cycle assessments

Currently only a limited number of LCAs exist in the literature, which cover lithium-ion vehicle batteries, and data sharing occurs amongst many of these. The CO_2 emissions results of the main assessments identified are presented in Table 3.2, which shows there are differences of (up to) five-fold, in the impacts reported per kg of battery manufactured.

Study	Battery type	kg of CO ₂ produced per kg of
		battery manufactured
Majeau-Bettez, et al. 2011	NCM, LFP	22, 22
Notter, et al. 2010	LMO	6
Zackrisson, et al. 2010	LFP, water as solvent	16
Zackrisson, et al. 2010	LFP, NMP as solvent	25
Dunn, et al. 2012a	LMO	5

Table 3.2 Results of existing lithium-ion battery LCAs

This degree of variation is so large that it can radically affect the whole life findings of vehicle comparisons. To show this, Figure 3.3 was constructed using the impacts reported in Notter, et al. (2010) and Zackrisson, et al. (2010), to model the low and high values respectively for the production of a 24kWh electric vehicle battery pack. The same parameters given for Figure 2.4 were employed, with the assumptions of a 150,000km vehicle lifetime and average EU electricity mix emissions during operation. Data for the vehicle production was taken from Volkswagen AG, (2008). The BEV production, excluding the batteries, was modelled using the CO_{2e} impacts of a petrol vehicle, based on the findings of Notter, et al. (2010), which indicated the values were similar.

Figure 3.3 indicates how the emissions of BEVs could significantly change, depending solely on the battery production impacts employed and how this can alter comparisons against an efficient ICE vehicle.

To help establish the reasons for these variations the following section reviews the methodology, data and assumptions used in the assessments given in Table 3.2. This is followed by an outline of some of the common findings and limitations identified. Finally, LCAs which cover battery recycling are addressed.

To avoid repetition, some of the more specific details of these assessments are discussed in Chapter 4, which compiles the inventory for the new battery LCA developed in this thesis.



BEVs are assumed to require one battery replacement to equal ICE vehicle lifetime.

Figure 3.3 Influences of battery production impacts

3.4.1. Battery manufacturing life cycle assessments

The assessment conducted by Majeau-Bettez, et al. (2011) incorporates LCAs for a NCM and a LFP battery pack. They provide a substantial inventory for the materials used. However, the value used for the manufacturing energy was taken directly from an earlier report by Rydh and Sanden (2005), which itself referenced a further document that could not be accessed. This assumption had a major impact on the findings, resulting in approximately 6kg of CO_{2e} per kg of battery, for the manufacturing alone, which is higher than the total value quoted by Dunn, et al. (2012a).

Their results showed that the NCM pack exhibited lower production emissions on a per kWh basis than the LFP one, but that the results were reversed when cycle life was considered in the functional unit. This resulted from the LFP cells being modelled with a much higher cycle life than the NCM variants (6000 cycles appose to 3000).

Some of the key findings of the assessment were that:

- Polytetrafluoroethylene (PTFE), used as a binder in the electrodes, is a key contributor representing the majority of the ozone depletion emissions and a significant proportion of the CO_{2e} value.
- The production of the battery management system contributes, approximately 10% to 30% of most impact categories.
- There is a shortage of data, regarding the energy consumed in manufacturing batteries.

The LCA conducted by Notter, et al. (2010), forms the basis of the lithium-ion battery inventories supplied within the Ecoinvent database (Ecoinvent, 2012). It details the production of a LMO lithium-ion battery and the accompanying supporting information provides a comprehensive breakdown of the inventories, which enables the input flows and assumptions to be checked.

Their results showed that the cells were responsible for approximately 73% of the total battery pack impacts and that the aluminium used in the cathode was a major contributor, representing 21% of the CO_{2e} emissions and 16% of the energy demand.

Review of the inventory however revealed, that compared to other cells, the cathode mass may have been underestimated and the anode overestimated (Zackrisson, et al. 2010; Majeau-Bettez, et al. 2011; Nelson, et al. 2011a). Given that the cathode was shown to already represent over 36% of the total CO_{2e} emissions, this discrepancy could have resulted in a significant underestimation of the total impacts. Further evidence for this can be derived from their suggestion that, one of the reasons the impact results are low is due to the batteries only containing a total of 7 grams of lithium, per kg of battery. Using equation (2.7) and a LMO cell voltage of 3.8V (Element Energy, 2012), this amount of lithium is theoretically only capable of allowing the battery to produce 103Wh/kg. This is already below the value of 114Wh/kg used in the report and will be further reduced by in efficiencies and lithium contained in the electrolyte.

The LCA of a LFP battery pack by Zackrisson, et al. (2010), focused on the effects of replacing the traditional polyvinylidene fluoride (PVDF) binders, which require N-methyl-2-pyrrolidone (NMP) solvent, with an option that utilised water.

This substitution of the solvent and binder was shown to reduce the total production CO_{2e} emissions by 37%, indicating this one assumption can have a huge effect on the results. However proxy data, which had exceptionally high production impacts, was used for PVDF and the NMP binder was modelled as being burnt off resulting in CO_{2e} emissions. Other sources suggest that most of the NMP is recovered for reuse, with possibly only half a per cent being burnt (Nelson, et al. 2011b). Subsequently, the report may have overestimated the impacts of the PVDF binder and solvent.

To approximate the assembly energy they divided the total energy usage reported by the battery manufacturer, Saft, by the company"s revenue and then multiplied it by the price of lithium-ion batteries. This gave an assembly requirement for the cells, modules and pack,

of 11.7kWh of electricity and 8.8kWh of natural gas per kg of battery produced. Unlike most other assessments that are based on theoretical calculations or proxies, this method has the advantage of incorporating actual process data. However, Saft produces a variety of battery types, with different production volumes and potentially conduct other operations as well (Saft, 2009). The scope is also unclear which introduces significant speculation as to how representative of mass lithium-ion battery production the values are. Based on these values, Zackrisson, et al. (2010) results indicated that the assembly was responsible for half of the total GHG emissions, which shows that it could be extremely important, but further work is needed to verify the approximations they have used.

Dunn, et al. (2012a) highlighted the discrepancies amongst assessments, discussed above, and suggested one of their aims was to resolve this. The assessment included a beneficial sensitivity analysis and was designed to form part of the GREET model and uses the data contained within, along with new inventories derived for the major battery materials. This has the advantage of providing data that can be contrasted with that of Ecoinvent, which was used in all the battery assessments discussed above, to help establish any potential errors. However, the production impacts of many minor materials, e.g. lithium fluoride which is used as a precursor for the electrolyte production, were omitted in the model.

They suggested that the battery assembly energy, and the way it is calculated, is responsible for much of the discrepancy found amongst the results of existing assessments. From their results they concluded that battery assembly is only a minor contributor, accounting for no more than 6% of the total energy consumption or GHG emissions. This is in contrast to the far higher values given in Zackrisson, et al. (2010) and Majeau-Bettez, et al. (2011). However, the primary energy consumption resulting from battery assembly in Dunn, et al. (2012a) was found to be 6.5MJ/kg (using the GREET model), which is over 6% of the figure they quote for the total battery. Along with this, the assembly energy was found to be based on the assumption that the dry room and formation/cycling steps constituted 60% of the total assembly energy requirements. The dry room requirements were based on further work by the authors (Dunn, et al. 2012b), in which natural gas was the main energy input, but this appears to have been omitted with only an electricity requirement included in the later assessment. This coupled with checks of their energy calculations for the formation/cycling steps, which revealed further potential inconsistencies, indicated caution should be observed when interpreting the results and that further work is needed.

Common consensus and limitations

Despite the discrepancies in their final results, several trends were seen amongst the findings. Some of the most prominent were that:

- The BMS is a key contributor to the overall impacts, typically adding over 10% of GHG emissions, although they were modelled as only representing 3%, or less, of the mass.
- The production of the cathode active materials and aluminium (used for example as the cathode substrate and cell container) are both large contributors to the impacts.
- The input lithium required is not indicated to be one of the major sources of impacts. With the exception of extraction from sea water, which is presently an unlikely option, this has been shown to be the case for different lithium sources (e.g. brines or ores) and locations (Dunn, et al. 2012a; Stamp, et al. 2012).

The assembly impacts were found to be a major source of discrepancies, with suggestions ranging from them being the main source to only a minor contributor. The scope of what is included in the assembly is unclear though, which may be responsible for some of this variation. The reports that indicated low assembly energies aimed at quantifying the requirements for the main individual operations. There can however be significant additional requirements associated with manufacturing processes, which may be overlooked. These additions, such as cooling, oiling, temperature control, machine idling and work handling, can in some cases have higher total requirements than the actual task modelled e.g. material removal (Gutowski, at al. 2006). The high assembly energy reported by Zackrisson, et al. (2010) was based on the total requirements for a manufacturer. This may have included all these additional consumptions, along with others associated with a complete manufacturing facility, such as lighting, heating and research and development operations, which may account for some of the higher values.

Several additional areas were also found to be potential causes of variations in all the assessments. Some of the most significant were the proportion of the battery pack that the cells constitute, the inventory used to model the anode and production losses.

The cells have typically been modelled as representing approximately 80% of the total pack mass. A review of packs used in BEVs however, shows they currently represent a much smaller proportion, see Table 3.3. This puts the cell mass nearer 60% of the total, which will alter the relative material constituents and therefore the production impacts. The

pack storage capacity is controlled by the cells. Therefore changes in their mass will also affect the pack capacity, which in turn will impact the vehicle. For example, a lower cell mass fraction will result in a heavier pack for a given storage capacity, which will increase vehicle energy consumption.

Pack	Cell mass	Cells per	Total pack	Cell % of total
	(kg)	pack	mass (kg)	pack mass
Nissan Leaf	0.799	192	292	53
Mitsubishi i-MiEV	1.7	88	235	64
EnerDel 19.6kWh BEV	0.449	336	263	57
Battery Pack				

(Lithium Energy Japan, 2010; EnerDel, 2012; Ikezoe, et al. 2012)

Table 3.3 Approximate cell proportions of various battery packs

Alternative designs may be able to produce packs with cell masses nearer those used in existing assessments. However, much of the additional mass comes from the casing which usually has to be substantial enough to support the large mass of cells and provide protection e.g. prevent water ingress, restrict movement, such as twisting that could lead to internal short circuits, and ensure safety during crashes.

Dunn, et al. (2012a) state that their results show the production of the graphite, used as the anode active material, is not a major contributor to the impacts, although it represents 8% of the energy consumption. Their inventory, along with that of Majeau-Bettez, et al. (2011), appears to use the energy requirements for producing baked carbon anodes as a proxy for the graphitisation process. This process has significantly lower energy requirements and temperatures (ECGA, 2012). Given that graphite represents about 15% of the cell mass, this could have a noticeable impact on the results. The graphite inventory (Ecoinvent dataset for battery grade graphite) used by Notter, et al. (2010) and Zackrisson, et al. (2010), models the graphitisation process using calculations based on the material specific heat capacity and required temperature. However, there are many other materials/processes involved that are not accounted for (DOE, 2010a). The inventory also seems to be an inconsistent mix between both the artificial and natural graphite production routes (Hawley, 2012).

Details concerning manufacturing losses were, on the whole, found to be limited in the existing literature. Notter, et al. (2010) did include losses, but they often used estimates due to limited data availability.

3.4.2. Recycling

Life cycle assessments covering the recycling of lithium-ion batteries are even more limited in the literature than those of their production (Sullivan and Gaines 2012). This situation is further complicated by different recycling routes (see Section 2.3.2), input materials (i.e. lithium-ion cell type), recovery amounts and types of output materials, e.g. pure metals or carbonates (Xu, et al. 2008; Gaines, et al. 2011).

The reports that are available indicate that recycling could have substantial benefits (Fisher, 2006; Dewulf, et al. 2010; Dunn, et al. 2012a). For example, Dewulf, et al. (2010) showed how the use of recycled nickel and cobalt can reduce demands and Dunn, et al. (2012a) indicated the potential benefits of recycling the cathode materials via several routes. Of these routes, a hydrometallurgical process for LMO cathode material (see Section 2.3.2) was shown to only offer limited benefits. This was due to the input requirements for the recycling process and the fact that much of the energy was consumed during the syntheses of the cathode material, rather than the precursors that are reclaimed. A further route they analysed involved recovering materials that can be directly reused in batteries, with little additional processing. This option showed over a 75% reduction in the cathode manufacturing energy, because both the processing and material requirements were abated. However, the process is not commercialised and questions remain as to whether the reclaimed materials will exhibit the same performances as those from primary sources (Dunn, et al. 2012b).

The majority of the existing work focuses on recovery of metals, which can potentially offer large recycling benefits, with other materials and the impacts associated with separating/sorting complete battery packs prior to reclamation often being overlooked.

3.5. Effects of battery parameters

How and what battery parameters are incorporated into LCAs of electric vehicles have been identified as a source of discrepancies amongst assessments (Matheys, et al. 2007; Majeau-Bettez, et al. 2011). The main parameters that need to be considered are battery mass, permissible DOD, lifetime, range and energy efficiency, which are discussed in Section 2.3.1. Accounting for these factors, Gerssen-Gondelach and Faaij (2012), showed that the energy consumption of a BEV using many advanced batteries, (e.g. lithium-air and lithium-sulphur) may be higher, despite their far greater specific energies. This arises from their lower energy efficiencies, compared to lithium-ion batteries, offsetting the gains of their reduced masses. Only for some long range BEVs, where the significant mass of lithium-ion batteries dramatically increased the vehicles energy consumption, were gains shown for the advanced batteries. However, the assessment did not consider the battery production or recycling phases. The battery LCA conducted by Majeau-Bettez, et al. (2011) also evaluated some of these factors and showed that cycle life differences amongst lithium-ion batteries have a large bearing on the results.

3.6. Summary

Many assessments of alternative powertrains were found in the literature. However, the majority of the focus has surrounded the WTW phases of vehicles. Assessments that covered vehicle production, and more specifically that of BEVs, were found to be far fewer and typically presented values for a single fixed lithium-ion battery.

The results of comparisons between powertrains were found to be greatly affected by factors such as the inclusion of the production impacts, the driving cycle used and the vehicles contrasted.

The review of battery production LCAs showed that, although several studies have been produced which provide a good basis, there is still a large degree of uncertainty regarding the results. The benefits and limitations, found in all the assessments, mean it is difficult to conclude which values are likely to be closest to those for actual battery production, which itself is subject to differences. This leaves LCAs of BEVs open to much variability, as shown in Figure 3.3. Many of the limitations found (e.g. variations in the assembly energy and production impacts of specialist materials), result from a scarcity of data on actual processes used to manufacture batteries, which may be difficult to overcome at present.

The results of existing assessments, given in Table 3.2, would seem to indicate that LMO batteries have far lower impacts than NCM and LFP variants. This may be true to some extent, however much of the discrepancy is expected to have resulted from differing assumptions used in the assessments.

Several works were identified that have begun to establish the effects of battery parameters, such as efficiency and mass, on the impacts of BEVs. However, limited research was found that encompass the influences of these, in conjunction with those of vehicle production and use, particularly for variations amongst lithium-ion chemistries.

The review revealed that, to permit improved LCAs of BEVs, significant work is needed to better understand the influences of their batteries. Specifically this requires:

- Resolution of the discrepancies amongst battery LCAs and how variations in the chemistry affect the results.
- Quantification of the end-of-life processing impacts of whole battery packs.
- Integration of battery parameters into LCAs, which also incorporate the production and use phases, to enable studies of their effects on the lifetime impacts of BEVs.

4. DEVELOPMENT OF AN IMPROVED LITHIUM-ION BATTERY LCA

4.1. Methodology

This chapter describes the battery life cycle inventory compiled to evaluate the discrepancies found amongst existing assessments and to study the effects of battery parameters.

It has been structured in the life cycle assessment (LCA) format, as laid out in ISO 14040, specifically covering the first two parts, "Definition of the goals and scope" and "Inventory analysis", see Section 3.2.1. However rather than simply compiling a list of flows, the data used in existing assessments was also investigated and discussed. This was performed to help identify any assumptions or inaccuracies that could introduce significant discrepancies in the results. The derivation of some of the inventories involved a significant amount of discussion on the processes and precursors. This data has been incorporated because it is important for the transparency of the LCA, in order to permit any assumptions used to be checked and to help ensure the results are correctly interpreted (British Standards Institution, 2006a).

The assessment was initially constructed to model the production of a Lithium manganese oxide (LMO) battery and was subsequently expanded to encompass the end-of-life (EoL) phase and other lithium-ion cathode materials. Throughout the model key variables were parameterised to allow the effects of the assumptions used to be studied. To compile the overall inventory and supply background data, the specialist software GaBi 6 was used.

The results of the model and discussion of the findings are provided in Chapter 6.

4.2. Assessment goals

The aim of this LCA was to quantify the effects of batteries and to help identify optimal trade-offs between components/parameters.

The objectives of this model were to:

- Examine and resolve the inconsistences in current LCAs of lithium-ion battery production.
- Include and quantify the impacts of battery recycling for which limited data is currently available.

- Identify the most significant processes and materials in the production/recycling of batteries.
- Identify areas where data limitations or variations (i.e. different processing options) could potentially have a significant bearing on the overall results.
- Assess the differences in impacts arising from lithium-ion batteries with alternative cathode materials.
- Generate a parameterised battery LCA that can be integrated with further models to enable whole life impact assessments of battery electric vehicles (BEV).

4.3. Assessment scope

4.3.1. Functional unit

In this chapter the functional unit for the analysis was based around the production and end-of-life (EoL) processing of one kg of lithium-ion battery pack.

The choice of a mass basis for the functional unit in this chapter was chosen to assist compilation of the inventory and aid comparisons with the results of other battery LCAs. The values were subsequently converted into an energy basis, using multiples corresponding to the parameters for each of the battery chemistries, to attain data for the vehicle level assessment given in Chapter 5.

Lithium-ion battery packs can vary depending upon, for example, the particular cell chemistry used and their intended application. In this assessment details for battery packs suitable for use in a "C"segment BEV were used, i.e. high energy packs with capacities in the region of 24kWh (Ikezoe, et al. 2012). To encompass some of the possible lithium-ion cell chemistries, three variants, identified as currently being the most feasible options for BEVs (see Section 2.3.2), were included in the assessment. These were LMO, lithium iron phosphate (LFP) and nickel cobalt manganese (NCM), named after the cathode material they utilise. All the batteries were assumed to use graphite anodes.

4.3.2. Assessment boundaries

The life cycle inventory (LCI) presented in the following sections encapsulated the production and EoL impacts associated with a vehicle battery pack, as shown in Figure 4.1. The EoL inventory was segregated to allow for assessments with and without the effects of recycling to be conducted.



Figure 4.1 Processes considered in the battery assessment

The production phase covers the steps up until the point the battery pack is ready for incorporation into a vehicle, specifically encapsulating:

- Extraction of raw materials.
- Processing of raw materials.
- The energy requirements for manufacturing the components and final battery pack.
- Manufacturing losses and their EoL treatment.
- Transportation of materials and components. Due to the low masses usually involved, transportation of manufacturing scrap to EoL facilities has been omitted.
- The cell formation and testing cycles.

The EoL phase includes:

- Removal of the battery pack from the vehicle and disassembly.
- Recycling of the non-cell pack components.
- The requirements for separating and sorting the cells into material streams for further processing.
- EoL processing of the cell material streams.
- Credits for the avoided burdens of the reclaimed materials.
- Transportation of materials.

Factors that have not been covered in this assessment are the impacts associated with:

- Research and development operations.
- Transportation of the workforce.
- Administration e.g. sales and marketing.

- Construction/maintenance of the necessary facilities and machinery (some impacts from these aspects are however present in input datasets).
- The use phase (this is incorporated later in Chapter 5).

Cut-off criteria

All identified processes and flows were included but, for practicality reasons, values were excluded where no data was available and their influences were judged to have marginal impacts, taken as <0.5%, of the overall GHG results. For potentially significant process or input flows, where data was unavailable, best estimates have been used to fill gaps. In such cases reference was made in the inventory to permit sensitivity analysis of the assumptions, if they were anticipated to have a significant bearing on the overall results.

Details on the cut-off criteria used in the GaBi background data can be found in Baitz, et al. (2011).

4.3.3. Impact categories

The main impact category evaluated in the assessment was global warming potential (excluding biogenic carbon which is assumed to be cancelled out by that absorbed by crop growth). This was calculated using the methodology compiled by the Institute of Environmental Science (CML) at Leiden University (Netherlands) based on a timeframe of 100 years, which was provided within GaBi 6. This method converted different emissions into carbon dioxide equivalents (CO_{2e}), using multiples based on their impacts relative to CO_2 . For example, methane has a characterization factor of 25, meaning it results in 25 times the impacts of CO_2 over a 100 year timeframe.

Due to data limitations and the variability found in the CO_{2e} findings, for which more information was generally available than other impacts, the assessment was focussed on GHG emissions. This was to enable improved quantification and understanding of GHG emissions, rather than generating figures for many impact categories whose results are anticipated to be extremely subjective. The assessment is therefore not a full LCA. However the model was used to calculate primary energy consumption and other impacts to give an idea of approximate trends.

4.3.4. Data requirements

This section describes the sources and methods used to select the inventory data.

Data sources

Primary data from manufacturers on the production of lithium-ion batteries was found to be limited. To overcome this, the majority of the production data was sourced from the available literature. However, to minimise any discrepancies resulting from this data, inputs were verified against multiples sources and similar processes to ensure they were representative. This allowed the most suitable data to be employed, or new inventories to be generated for significant processes, if those available were found to be variable or unrepresentative.

However it should be noted that variability will still exist. This can result from, for example, discrepancies in the precise processes employed by various manufacturers (Kendrick, 2013), different production volumes and developments in batteries and their manufacturing techniques.

Primary data was used to model the end-of-life phase and supplemented with literature values as necessary. This provided useful data based on actual recycling operations which helped fill gaps in the existing literature. However, due to confidentiality reasons, only aggregated data is presented to disguise the precise process and values.

The background data was sourced firstly from the GaBi 6 database. If sufficiently accurate or representative datasets were not available, data from Ecoinvent V2.2 was used (Ecoinvent, 2012). Finally, if this did not identify suitable data, new inventories were derived based on "best" available sources or proxies used if the factor being substituted was judged to have minimal effects on the results.

Data coverage

Processes have been assumed to occur in Europe as a default. Therefore, where representative datasets were available, inventories for average European processes were used. For processes known to occur outside Europe, data for the main country of origin have been used including that for any inputs e.g. electricity.

The technology/processes used to manufacture batteries vary as noted in the previous section. Where data was available this assessment aimed to model the most common or viable routes identified at the time of compiling the inventory. The values therefore represent approximate averages for production around 2013.

The technology modelled for the EoL phase is also representative of 2013, but specifically refers to a hydrometallurgical process for the cell treatment (see Section 2.3.2). Non-cell components were treated in line with relevant common industry processes.

Data precision

The data used to populate the LCI model was inputted to the greatest level of precision that was attainable or practical, generally up to three significant figures. This practice does not mean that the data is precise to this level, but has been employed to help with mass balances and minimise the introduction of any compounding errors caused by rounding in multiple calculations.

Knowledge of the uncertainties associated with many of the values is limited. However where potentially large deviations were identified, e.g. multiple processing routes which may have drastically different impacts, discussions were included in the relevant sections.

Allocation

Where a process yielded co-products along with those desired in the assessment, system expansion was used as recommended in ISO 14044. This was performed by crediting the co-products with avoided burdens related to the materials they substitute.

4.3.5. Life cycle inventory methodology

In this section the methodology followed to compile the LCI is outlined. This includes the main assumptions used to address areas such as transport and wastes. Assumptions necessitated in specific processes are detailed in the relevant inventory sections.

Transportation

For products and materials which were manufactured in Europe a default transportation distance of 500km by truck was employed. This was modelled using GaBi data for a 22 tonne payload truck and average EU diesel, in line with the scope given in Section 4.3.4. The model was parameterised to allow the effects of this assumption to be assessed.

For products produced elsewhere, transportation to Europe was estimated according to the country of origin. To account for subsequent transportation from a drop-off point (e.g. port or station) the same parameterised truck model covering 500km, used for products within Europe, was also included.

To permit evaluation of the additional transportation impacts, all the associated inputs were grouped within GaBi. This grouping did not include transportation incorporated in the background input processes.

Energy inputs

Average European electricity and heat inputs have been used, unless the process was known to occur outside Europe. The specific default GaBi datasets employed were "EU-27: Electricity grid mix" and "EU-27: Thermal energy from natural gas". Due to the large variations in grid emissions between plants and locations, which are discussed further in Chapter 7, it should be appreciated that production using electricity grids which differ significantly from the EU average will affect the results.

Wastes

Details of the specific waste treatments applied are given in the relevant inventory sections. The following general assumptions were used based on common processing options:

- Metals recycling including credits for avoided burdens of primary production.
- Plastics incineration or granulation/recovery with credits for avoided burdens for larger quantities of unmixed plastics. Some incineration is used to produce electricity and/or heat. Electricity credits were given for large waste streams in the EoL phase but, due to the small amounts involved, none were given for production waste incineration.
- Carbon materials at EoL incineration with energy recovery or landfill.
- Other materials landfill.

Assembly impacts

Establishing the battery assembly requirements and their influences on the impacts has proved problematic in many previous LCAs, see Section 3.4.1. It is often not possible or is difficult to segregate them from those of the input materials and variation exists regarding what processes are included, which hampers comparisons between assessments.

Despite these limitations it is still useful to provide an approximation of what impacts result from the specific processes used to assemble battery packs, in order to identify hotspots. Therefore, the model was parameterised to allow the influences to be segregated from those of the input materials/components. The scope for the assembly impacts was taken to encompass the energy and machinery consumables (e.g. cooling air) used for pack assembly, cell assembly, cell container shaping and electrode production (e.g. mixing, coating, drying and shaping). Further details of these can be found in the relevant inventory sections. Material losses (e.g. cell container offcuts and the solvents used during the electrode coating) and specialist material processing requirements (e.g. manufacturing of the active powders) were not include in the assembly impacts. Note the value is different to those given for final cell and battery pack assembly, Sections 4.4.8 and 4.4.11 respectively, which each only include a subset of the total assembly requirements.

Production methodology

The mass percentages of the complete cells and other main components were defined based on in-house measurements and values in the existing literature. Further details are given in Section 4.4. The values were assumed to be constant for all the cell chemistries assessed. These percentages will vary due to differences between cells and manufacturers for example. Therefore the model was parameterised to permit sensitivity analysis of the values.

To calculate the mass percentages of the cell constituents, data from Argonne National Laboratory"s Battery Performance and Cost model (BatPaC) was used (Nelson, et al. 2011a; Nelson, et al. 2011b). This model was chosen because it provided a good level of detail, had been peer-reviewed by industry, was publicly available, modelled several different chemistries and permitted batteries to be tailored to a specific task (e.g. for BEV or PHEV applications). For the cells used in this assessment the model was set to provide data for a BEV battery pack with a capacity of 24kWh and power of 90kW. These values were chosen to approximate the size of battery packs currently fitted to "C" segment electric vehicles, as defined in the functional unit.

The cells modelled using BatPaC and their corresponding specific energies, which refer directly to the cells modelled to minimise discrepancies, are given in Table 4.1.

Name	LMO	NCM	LFP
Cathode composition	LiMn ₂ O ₄	$Li_{1.05}(Ni_{4/9} Mn_{4/9} Co_{1/9})_{0.95}O_2$	LiFePO ₄
Cell specific energy Wh/kg	153	204	141

Table 4.1 Specifications of cells modelled

The BatPaC model was based on projections for 2020 (Nelson, et al. 2011b). Comparison of the LMO results against those used for a battery pack of comparable capacity and chemistry in the Nissan Leaf, revealed similar specific energy at the cell level. The higher values reported for the NCM cells may however represent state-of-the-art values and possibly be more representative of those attained in the next series of BEVs (Element Energy, 2012). At the pack level differences were evident with the relative mass of the non-cell components appearing to be lower than in current BEVs, see Section 4.4.1. Therefore, data from BatPaC was only used for the cells.

The derived material percentages were verified against primary data for the outputs of electric vehicle battery pack recycling.

The inventories were initially derived based on LMO cells which are employed in many current EVs, such as the Nissan Leaf and Chevrolet Volt (Duong, 2010). With the exception of the cathode material it was assumed that all the cell constituents could be utilised in the other chemistries assessed (Lowe, et al. 2010; Majeau-Bettez, et al. 2011; Nelson, et al. 2011b). Excluding the cathode, this allowed the NCM and LFP cells to be modelled using the same inventories, although with differing mass percentages.

End-of-life methodology

To assess the impact of the EoL phase the avoided burdens approach (or end-of-life approach) was used. This method involves applying credits for recycling at EoL, corresponding to the avoided burdens of the outputs, and applying impacts for scrap used during materials production (World Steel Association, 2011). This methodology was chosen to allow easy segregation of the recycling impacts, thereby permitting a scenario without recycling to be modelled.

Recycled materials from electric vehicle (EV) batteries will not be available for incorporation into new packs until the first generation of EVs reach their EoL. Average vehicle lifetimes are currently around 13 years so, depending upon the lifespan of EV batteries, there will be a significant time lag in the availability of recycled materials. This problem will be further exacerbated by growth in EV sales, changes in battery constituents as the technology matures and losses (e.g. recycling inefficiencies or batteries diverted for secondary usage). Therefore, the available percentage of recycled materials for manufacturing (i.e. effectively a closed-loop scenario assuming reclaimed materials are suitable for reincorporation into new batteries) will vary with time. This in turn will

influence the LCA results potentially resulting in over or under estimations, depending on the available and modelled recycled content, as discussed by Stasinopoulos, et al. (2012). Existing recycled materials from other applications could be utilised. However, this will affect other products and potentially lead to double counting of recycling benefits or shifting of burdens, because more primary materials are subsequently necessitated in other applications. The materials from end-of-life battery recycling are likely to enter general remanufacturing streams at some point and become mixed with other sources. However, this should not have a significant influence on the results, because the specific impacts from recycling battery materials are accounted for in the model and the flows of recycled materials to and from the wider system should balance.

4.4. Battery production inventory

In this section the inventories and their derivation are detailed, together with any specific limitations or assumptions employed. Firstly, those for the battery pack and cells are presented, followed by those for each of the constituents. Reference has also been made to existing assessments to help identify significant limitations and the reasons for discrepancies. This enabled the research to focus on generating improved inventories for these areas, thereby helping to fulfil the assessment objectives (see Section 4.2).

The process diagram for the cell production is given in Figure 4.2, and battery pack in Figure 4.3. These show each of the components that are addressed in the following subsections.



Figure 4.2 Process diagram for cell manufacturing



Figure 4.3 Process diagram for battery pack manufacturing

4.4.1. Battery pack constituents

The mass of car traction batteries can vary enormously. Currently though those fitted to "C"segment BEVs, as defined in the functional unit, such as the Nissan Leaf and Renault Fluence Z.E. are around 300kg (Renault, 2011).

The main existing LCAs of EV battery packs have taken the cells to represent approximately 80% of the total mass, see Section 3.4.1. However a review of packs used in EVs (see Table 3.3) showed the cells currently represent a much smaller proportion, approximately 50% to 70%, which matches the findings of Kwade and Bärwaldt (2012). The cells were therefore modelled as representing 60% of the total pack mass in this assessment.

To permit the influences of this assumption to be studied, the GaBi model was parameterised using equation (4.1). This allowed the relative mass percentages of all the non-cell components to be scaled by only varying the total non-cell mass percentage. This simple equation was deemed to be sufficient to judge the effects of practical changes in the cell mass percentage. However for high cell percentages, particularly >80%, it may result in unrealistic amounts for some of the components e.g. the battery management system (BMS).

Component mass =
$$(B_i/40)$$
*NNC (4.1)

Where:

 B_i = The base mass percentage for each of the non-cell components

NNC = The new (alternative) total non-cell mass percentage for the battery pack.

Based on the existing literature and measurements from a stripped down LiFeBATT 2E-108015 108V/15Ah battery pack, the approximate mass proportions used for the remainder of the pack were derived, see Table 4.2. The values given are based on an air cooled pack containing cells grouped into modules, which are encased in aluminium housings. These are in turn encapsulated in an outer housing constructed from steel and moulded plastic. It should be appreciated that this is just one of many possible variations. For example the use of liquid cooling, alterations to the cells or different module arrangements will all influence the materials and their masses.

Component	Material	Percentage
Cells		60
Module -casings	Aluminium sheet 0.5mm	5
Module – insulation/supports	Polypropylene moulding	3
Module -terminals threaded	Copper	1
Pack casing (steel)	Sheet steel	15
Pack (plastic)	Polypropylene mouldings 80% and	
	PVC 20%	10
Fixings	Stainless steel	1
Bus bars and terminals	Copper	0.5
Main cabling	High voltage insulated copper wiring	1.8
BMS (circuit boards only)	Circuit board	0.7
BMS (relays, sensors, fuses etc.)	Various	1
BMS wiring	Insulated copper wiring	1

Table 4.2 Battery pack mass percentages

4.4.2. Cell constituents

Table 4.3 shows the cell mass percentages derived from the BatPaC model (Nelson, et al. 2011a). The amounts refer to the contents in the finished cells and not those required for production which may differ due to manufacturing losses.

	Mass percentage		ge
Component	LMO	NCM	LFP
Cathode material	44.1	36.4	32.4
Anode material	15.3	23.1	16.9
Cathode foil (aluminium foil)	4.9	4.5	5.8
Anode foil (copper foil)	10.7	9.9	12.4
Separator	1.7	1.6	2
Electrolyte	14.3	14.8	20.9
Cathode terminal (aluminium sheet)	0.9	1	0.9
Anode terminal (copper sheet)	3	3.4	3
Cell container (laminated aluminium)	5.1	5.3	5.7

Table 4.3 Cell mass percentages

The values can vary for many reasons e.g. due to differences in the capacity of the active materials, the pack requirements and the permissible electrode thickness (Nelson, et al. 2011a). Therefore, as with the pack constituents, they are only approximations for one possible configuration and further variation can arise from any assumptions/estimates used to overcome data limitations.

To indicate the potential variations Table 4.4 was constructed. This shows the approximate mass percentages reported for LFP cells, for which the most data was identified in the existing literature.

	Mass percentage			
Component	Zackrisson, et al. 2010	Majeau-Bettez, et al. 2011	Gaustad, et al. 2012	Values used in this assessment
Cathode material (with binder/conductive aid)	51.3	31	23.9	32.4
Anode material (with binder/conductive aid)	19	10	17.2	16.9
Cathode foil/terminal	2	4.5	5.1	6.7
Anode foil/terminal	4.9	10.4	13.8	15.4
Separator	1.9	4.1	4.9	2
Electrolyte	19.6	15	10.9	20.9
Cell container	1.3	25	24.2	5.7

Table 4.4 Mass percentages reported for LFP cells

Coincidentally both the reports by Zackrisson, et al. (2010) and Majeau-Bettez, et al. (2011) used data based on estimates given in Gaines and Cuenca, (2000), which makes the large variations between their findings surprising. This variation and a lack of further information, on the initial data sources for these assessments, make judgment of how representative the values may be of actual modern cells speculative. Comparisons with the mass values reported in these assessments were subsequently limited to avoid the introduction of potential discrepancies. However, both the assessments use the values to compile battery LCAs and the differing mass percentages they use will have impacted on their results.

The values given by Gaustad, et al. (2012) were derived following the dismantling of an LFP cell. The values refer to cylindrical 18650 cells, used in power tools with steel cases,

appose to laminated aluminium pouch cells often used in electric vehicles and modelled in this assessment. This difference in casing and the larger size of typical BEV pouch cells would explain the higher container mass percentage reported by Gaustad, et al. (2012). Attributing a larger proportion of mass to the container will lower the values of the other components, which is seen as the general case compared to the values used in this assessment. The exceptions to this are the separator and anode material. Data on the precise materials used in the cell examined in Gaustad, et al. (2012) is limited, but differences in these and the cell design may explain the variations shown. Compared to the other assessments, shown in Table 4.4, the ratio of the cathode to anode material masses is much lower in Gaustad, et al. (2012), but it is by far closest to the value for the data used in this assessment.

Considering the discussion above, the comparison with the primary data reported in Gaustad, et al. (2012) suggests the cell mass percentages used in this assessment are reasonable. The potential sources of variation should be appreciated though along with the discrepancies between the values assumed in other LCAs.

4.4.3. Anode production

This section describes the methodology used to model the anode production and the subsections provide further details on the active material.

The inventory used to model the anode is given in Table 4.5 and serves as an example of the format used for the other constituents modelled. It shows:

- The components used and what materials have been used to model them.
- The mass required per kg of final product.
- The background datasets used in the model. Unless otherwise stated data is from GaBi.
- Any additional important considerations, such as losses modelled or assumptions employed.

The processing losses were based on estimates for the mixing, coating, slitting, and stacking of the electrodes (Nelson, et al. 2011a; Nelson, et al. 2011b). An input of deionised water was included to model the solvent and the anode material percentage, given in Table 4.3, was taken to consist of 95% graphite and 5% binder.

Inputs (component/	Amount	LCI data used	Notes
material)			
Current collector -	446 g	Copper mix from	Including 8% loss
copper foil		electrolysis	
Active material -	609 g	See following	Including 8% loss
graphite		subsections	
Binder - styrene	32.1 g	Styrene butadiene	Including 8% loss (see
butadiene rubber		rubber mix	note below)
Solvent – deionised	1.6 kg	Deionised water	Mass ratio of 50:1 against
water			binder (Fan, et al. 2009)
Electricity	18.2 MJ	Default data, see	See below
		Section 4.3.5	
Outputs			
Anode - coated foil	1000 g		
Waste - graphite	48.7 g	Landfill of inert matter	
Waste - copper	35.7 g	Credit for recycling	See note below
Waste - binder	2.6 g	Incineration –waste	
		incineration of plastics	
		(PE, PP, PS, PB)	
Water vapour	1.6 kg	Elementary flow to air	
Waste heat	8.5 MJ		

 Table 4.5 Anode inventory per kg produced

Styrene butadiene was selected over traditional binders such as polyvinylidene fluoride (PVDF) and polytetrafluoroethylene (PTFE) because of the cost, production and environmental benefits it offers, which have prompted its increasing usage. Some of these benefits result from the use of water as a solvent instead of the N-methyl-2-pyrrolidone (NMP) used by PVDF, which is hazardous. This selection will alter the manufacturing requirements, as well as the input materials, which could lead to differences compared to other assessments which model more traditional binders, as shown by Zackrisson, et al. (2010), see Section 3.4.1.

To estimate the benefits of recycling the copper offcuts from anode production (see Table 4.5), a credit equal to the difference between primary copper production and that for copper containing 95% recycled content was applied.

The energy consumption was calculated from estimates for mixing and coating of the anode paste, followed by drying, rolling, slitting and notching to produce the final anode ready for incorporation into the cells (Nelson, et al. 2011a; Väyrynen and Salminen, 2012). Specifically the energy required to coat and dry 1kg of anode was calculated as 12.6MJ, using data for a lithium-ion battery continuous coating machine (Gelon LIB Group, 2013). This value was based on the size of the copper substrate per kg of anode and machine details of a feed rate of 2m/minute, processing width of 180mm and energy consumption of 20kW. The theoretical minimum energy for drying was calculated as 3.9MJ, based on the requirements to heat the anode to 100°C and vaporise the solvent. This suggests that the estimated value contains significant additional energy for the coating stage and the losses/additional requirements (e.g. conveyors and extractors) associated with the drying operation. Details on the other operations necessary for the anode production are given in Table 4.6. These gave a total energy requirement of 16.7MJ per kg of anode or 18.2MJ allowing for the 8% losses shown in Table 4.5.

Operation	Machine data	Operation duration	Energy
			MJ
Mixing	Mixer - 1250W 5 litre	Estimate for mixing binder/solvent	1
	capacity	(1.51) for 20 minutes and active	
		material/binder (1.8 litres) for 20	
		minutes (Huang and Wu, 2012)	
Coating	Continuous coating	See above text	12.6
and drying	machine		
Rolling	Continuous calendaring	Estimated 2 minutes operation based	1.8
	machine 15kW	on area of $12\mu m$ thick copper sheet	
		required per kg of anode, $\approx 3.8 \text{m}^2$.	
Slitting	Single sheet slitting	For 3.8m ² sheet 50 meters of slitting	0.2
	machine -750W	estimated, 5 min of operation at	
		10m/min.	
Notching	Automatic electrode	For 3.8m ² approximately 3 minutes	1.1
	forming machine 6kW	of operation.	
	(Gelon LIB Group, 2013)		
Total			16.7

Note values do not include the production losses given in Table 4.5.

Table 4.6 Anode production machinery electricity consumption per kg

Anode active material production

Several different materials can be used for the anode (e.g. lithium titanate and silicon) but graphite is currently the most common and has been used in this assessment (Cameán, et al. 2010). Review of available life cycle inventories revealed no suitable data for battery grade graphite, see Section 3.4.1. Due to this and the importance of graphite in lithium-ion batteries (\approx 15% of cell mass), new inventories were created.

Graphite can be produced from two routes, (i) via graphitisation of a carbon feedstock (artificial graphite), which is very energy intensive due to the high temperatures necessitated, $\approx 2800^{\circ}$ C, or (ii) through extraction from graphite containing rocks (natural graphite). Much of the graphite presently used for batteries is artificial, although in efforts to reduce costs natural graphite is being employed (Yoshio, et al. 2009; Cameán, et al. 2010; Wang, et al. 2012c). However, to improve the large irreversible capacity loss and poor cycling exhibited by natural graphite, significant processing (e.g. coating) is still necessary (Wang, et al. 2012c). Natural graphite has also been identified as a critical material, which raises issues for its use in mass battery production (European Commission, 2010).

Due to the large differences in the production routes between the two sources, it was decided to generate inventories for both. These are given in the following sections, together with that for the intermediate feedstock, found to be required during artificial graphite production. The model was then parameterised to allow the effects of the assumed source to be evaluated.

The main background report, employed for artificial graphite manufacturing, referred to a plant that was anticipated to use hydroelectricity because of the high energy consumption of graphitisation furnaces (DOE, 2010b). This is not the case for other plants (Graphite India Limited, 2007). Therefore the model was parameterised to allow the electricity supplied, for the graphitisation process, to be sourced from either the average European grid mix, which was assumed as the base case, or hydroelectricity.

The preliminary results for these options are given in Figure 4.4, together with those from existing assessments. This shows that the new inventories derived find substantially higher CO_{2e} emissions and that there may be significant discrepancies depending upon the source/production route assumed.



Figure 4.4 GHG emissions associated with battery graphite production

Natural graphite

The production of battery grade natural graphite involves the following steps (MEGA Graphite Incorporated, 2012; Shaw, 2012):

- 1. Extraction of rock containing ≈ 5 to 7% of the flake graphite required by batteries.
- 2. Sorting and crushing of the ore.
- 3. Liberation and concentration using a series of flotation cells and stirring.
- 4. Drying.
- 5. Sieving and milling, to produce the required shape. Only around 30-40% of the output is suitable as an anode material, with no practical use suggested for the balance (Northern Graphite, 2011). This is a high loss which may require further investigation.
- Further treatments/modifications to create the desired properties and remove impurities that could react with the electrolyte. For example high temperature heat treatments in inert atmospheres and coating (Zaghib, et al. 2003; Wang, et al. 2012c).

The impacts associated with these stages, were estimated as follows and are compiled in Table 4.7:

- Ecoinvent data for ,graphite at plant" was used to model the extraction and initial purification (Shaw, 2012). This dataset, although based on approximations, did not contain the additional inputs associated with the Ecoinvent dataset for ,,battery grade graphite", that were found to be potential sources of limitations, see Section 3.4.1.
- To allow for losses in the additional sizing and shaping of the input flake graphite a yield of 35% was assumed. The energy for shaping was based on data for milling to achieve an output size of 10µm (Larson, et al. 2012). This gave an electricity requirement of 229Wh per kg of anode (2.86kg of input material).
- Finally the energy requirements of a thermal purification step were applied (Takahashi, et al. 1996; Zaghib, et al. 2003). These were approximated using the electricity value of 1.93kWh (6.95MJ), found for the production of the intermediate material used in artificial graphite, which involves similar steps i.e. purification and the production of an inert atmosphere, see following section. The main impurities removed were suggested to be oxygen (approximately 1.4% of mass), aluminium and iron (Zaghib, et al. 2003). A corresponding flow of oxygen was therefore included to model the additional emissions, but due to their very low masses, the other materials were omitted.

Inputs	Amount	LCI data used	Notes
Flake graphite	2860 g	Ecoinvent dataset for	See note above
extraction		"graphite, at plant"	
Electricity	7.77 MJ	Modelled using estimate	Particle shaping and
		for China's grid mix	thermal purification
Outputs			
Graphite (natural)	1000 g		Battery grade
Waste graphite	1850 g	Landfill of inert matter	Unsuitable graphite from
			shaping process
Oxygen emission	14 g	Flow- Oxygen [Inorganic	Purification emission
		emissions to air]	
Waste heat	6.95 MJ		Heat from thermal
			purification

 Table 4.7 Inventory data for battery grade natural graphite
Most natural graphite is currently produced in China (European Commission, 2010). To account for this additional transportation of 20,000km by ship was applied and the electricity grid mix altered accordingly.

It should be noted that due to the assumptions used there is significant potential for variation in the data. Therefore improved data should be used to verify the results as it becomes available.

Artificial graphite

Artificial graphite can be produced from a variety of feedstocks. Petroleum coke is the most common base material and is produced from the heaviest portions of crude oil (Rand, 2003). Before use in the graphitisation process the petroleum coke is processed to obtain an intermediate material. This involves mixing with binders, such as petroleum or coal-tar pitches, and calcination to remove impurities (EPA, 1998; McChesney and Walden, 2011).

The data presented here was based on details for plants recently constructed in the US, for the specific purpose of large scale graphite production for battery anodes. To check the values obtained were reasonable, they were compared against data from a manufacturer of graphite electrodes for the iron and steel industries (Graphite India Limited, 2007).

The inventory for the intermediate material production is given in Table 4.8 and was calculated based on data given in DOE (2010a). The significant discrepancy in the mass balance is expected to have resulted from the unrecorded flows during combustion processes, e.g. oxygen and water.

The energy consumption listed for the intermediate material production from Graphite India Limited (2007), was approximately 2MJ/kg. This value is below that found in Table 4.8. However, the scope of this report did not encompass any of the processes prior to baking, e.g. mixing and shaping, which would account for some of the lower value.

The subsequent graphitisation process was based on DOE (2010b) and requires equipment such as cooling towers, dust collectors, screens, and conveyors along with electric graphitisation furnaces. No data was available on the quantity of final output material. Therefore an approximation was made based on the output of intermediate material from the facility which feeds the assessed graphitisation plant, minus the material lost in the emissions (DOE, 2010a; McChesney and Walden, 2011). The inventory is given in Table 4.9.

Inputs	Amount	LCI data used	
Xylene	656 g	Plastics Europe dataset available via GaBi	
Coke	948 g	Petrol coke at refinery	
Petroleum Pitch	711 g	Bitumen at refinery used as proxy - binder material	
River water (litres)	1400 1	Flow - River water	
Electricity	6.95MJ	Default data, see Section 4.3.5	
Outputs			
Graphite	1000g		
intermediate material			
Waste water cooling	1400 1	Flow - Water (river water from technosphere)	
PM ₁₀	2.2 g	Flow- Dust (PM2,5 - PM10) [Particles to air]	
VOC	0.25 g	Flow- VOC (unspecified) [Organic emissions to air]	
Organic hazardous	0.25 g	Flow- VOC, used as proxy.	
air pollutants			
CO ₂	1880 g	Flow- Carbon dioxide [Inorganic emissions to air]	
Non-hazardous solid	3 g	Landfill (Commercial waste for municipal disposal)	
municipal waste			
Non-hazardous solid	4 g	Landfill (Commercial waste for municipal disposal)	
waste off-site			

Table 4.8 Inventory for artificial graphite intermediate material

Inputs	Amount	LCI data used	
Intermediate material	1050 g	Graphite intermediate material see Table 4.8	
Electricity	24.1 MJ	Default data (average European grid mix) or	
		electricity from hydro power	
Outputs			
Graphite (artificial)	1000 g	Battery grade	
PM	1.59 g	Flow- Dust (PM2,5 - PM10) [Particles to air]	
СО	26.5 g	Flow - Carbon monoxide [Inorganic emissions to air]	
SO_2	0.33 g	Flow - Sulphur dioxide [Inorganic emissions to air]	
Hazardous air	0.58 g	Flow- VOC, used as proxy as they are likely to	
pollutants		represent the main constituents (EPA, 2010)	
Waste heat	24.1 MJ		

Table 4.9 Inventory for graphitisation process

Data for graphitisation from Graphite India Limited (2007), showed an electricity requirement of approximately 16MJ per kg. Considering the larger scale of this plant and potentially lower requirements (the output is intended for use in the iron and steel industries and not battery anodes), suggests the value calculated in Table 4.9 is likely to be a reasonable approximation.

4.4.4. Cathode production

The cathode losses, binder selection and methodology used to calculate the production energy requirements were based on the same assumptions as the anode, see Section 4.4.3. Adjustments were made to account for the higher active material loading and the densities of the materials. This gave a requirement of 16.3MJ per kg of cathode sheet, including 8% losses.

To help improve the conductivity of the active cathode material a conductive aid, typically carbon black, is added (Lux, et al. 2010). The data set used for carbon black refers to the process used to produce rubber and pigment grades. However the processes used to attain the high purity and properties, desired for lithium-ion batteries, are known to differ (Mitsubishi Chemical Corporation, 2013). Due to the low mass of carbon black in the overall model, this approximation should have a minimal impact on the final results.

The cathode material percentage given in Table 4.3 was further broken down into the following fractions; active material 0.89, conductive aid carbon black 0.06 and binder 0.05 (Lux, et al. 2010; Nelson, et al. 2011b).

Table 4.10 presents the inventory used for the LMO cathode manufacturing. This was subsequently adapted to account for the different active materials using the masses given in Table 4.3.

The following subsections detail the inventories derived for the three cathode active materials assessed, LMO, LFP and NCM.

Inputs	Amount	LCI data used
Current collector -	109 g	Aluminium foil (primary)
aluminium foil		
Active material - LMO	870 g	See following subsection
Binder - styrene	48.9 g	Styrene butadiene rubber mix
butadiene rubber		
Carbon black	58.7 g	Carbon black (furnace black; general purpose),
		see note above
Solvent – deionised	2.5 kg	Deionised water (Mass ratio of 50:1, (Fan, et
water		al. 2009))
Electricity	16.3 MJ	Default data
Outputs		
Cathode - coated foil	1000 g	
Waste – active material	69.6 g	Assumed to be treated in the same fashion as
		EoL waste see Section 4.5.4
Waste - aluminium	8.7 g	Aluminium foil - scrap credit
Waste - binder	3.9 g	Incineration –waste incineration of plastics
		(PE, PP, PS, PB)
Waste – carbon black	4.7 g	Landfill for inert matter
Water vapour	2.5 kg	GaBi elementary flow
Waste heat	12 MJ	

Table 4.10 Cathode inventory for LMO cell

Inventory for LMO cathode powder production

The variety of cathode materials used in lithium-ion batteries has resulted in existing LCAs modelling different chemistries. This not only complicates comparisons between assessments, but has resulted in exacerbating the deficiency in data for any particular chemistry. Two of the main LCAs available in the current literature (Notter, et al. 2010; Dunn, et al. 2012b), have evaluated $LiMn_2O_4$ production and this material was selected as the baseline in this assessment.

The situation is further complicated by a variety of potential production routes, materials sources, geographical locations and recycling effects (Stamp, et al. 2012). Figure 4.5 shows the results of existing assessments, which highlights the differences that some of these assumptions can make. The discrepancies between the results for primary production

may not be as large as for some materials, however considering the large mass the cathode active material constitutes, (around 25% of the final battery pack) the variations shown may still have as substantial impact on the final results.



Figure 4.5 Existing data for LiMn₂O₄ production

To try and establish the main contributors to $LiMn_2O_4$, and the reasons for the discrepancies given above, the manufacturing process has been reviewed below.

Common precursors in the existing literature for the syntheses of $LiMn_2O_4$ are lithium carbonate (Li_2CO_3) and manganese oxide (Mn_2O_3), which were subsequently selected for this assessment (Iwata, et al. 2001; Notter, et al. 2010; Cho, et al. 2012; Jung, et al. 2012).

Brines are currently the main source of lithium, although production from minerals also constitutes a significant share. Huge quantities of lithium are also contained in seawater. However the low concentrations, <0.2 parts per million, currently make it an impractical source (Mohr, et al. 2012; Stamp, et al. 2012).

This assessment has modelled lithium production from brines as the baseline, specifically Chilean brines, because they represent a large proportion of current production and are reported to contain over 30% of global reserves (Mohr, et al. 2012). However, lithium brine concentrations, depths, evaporation rates and extraction procedures/equipment vary significantly between locations, which could have substantial effects on the impacts as shown in Stamp, et al. (2012).

For the brine and subsequent Li_2CO_3 production impacts, in this assessment, data from Stamp, et al. (2012), for their "brine favourable conditions" scenario was used. This data was based on process information from the world"s largest lithium producer in Chile. The production process is multi-output, with the lithium brine being described as a by-product of potassium production, resulting in most of the impacts being allocated to potassium and not the lithium brine (SQM, 2011). Therefore, although currently a major source, this scenario may represent a low impact option, with higher impacts anticipated for other brine deposits with lower concentrations and different production allocations. The inventory has not been reproduced here, but can be found in the supplementary material accompanying Stamp, et al. (2012). Additional transportation of 14,000km was applied for shipping the Li_2CO_3 to Europe.

There has been much talk of possible lithium shortages resulting from the widespread use of lithium-ion batteries in vehicles. Several recent studies have concluded that sufficient resources exist to meet possible demands in the coming decades, and potentially in the far longer term, if high recycling rates are achieved or extraction from oceans becomes viable (Goonan, 2012; Kushnir and Sandén, 2012; Mohr, et al. 2012; Stamp, et al. 2012). However, potential supply issues could occur due to large demand increases and the majority of resources being concentrated in only a few countries. Kushnir and Sandén (2012) for example, concluded that a global initiative towards vehicles using lithium-ion batteries could leave them *"vulnerable to resources more concentrated than that of the oil supply system existing today*'. This underlines the importance of instigating an effective recycling infrastructure for lithium-ion batteries, to create a secondary source of lithium. Further assessment of supply was beyond the scope of this thesis. However, supply may be an important consideration if lithium-ion batteries were to be used extensively in global vehicles.

Manganese oxide (specifically Mn_2O_3) can be produced by roasting manganese carbonate in a kiln at temperatures above 400°C in the presents of oxygen (Kajiya and Tasaki, 2005). The process was modelled in Notter, et al. (2010) and Dunn, et al. (2012b) and the energy consumptions they reported are given in Table 4.11.

	Electricity kWh/ kg of Mn ₂ O ₃	Natural gas MJ/kg of Mn ₂ O ₃
Notter, et al. (2010)	0.005	4.13
Dunn, et al. (2012b)	0.023	2.91

Table 4.11 Literature values for manganese oxide production energy

No suitable process data was found from which to compile a new inventory. Therefore the data from Notter, et al. (2010) has been used in this assessment. This value represented the worst case scenario (of the options), which is consistent with GaBi modelling principles used for other datasets (Baitz, et al. 2011). However in this dataset the precursor to manganese oxide, manganese carbonate, was modelled using manganese concentrate which was found to have much lower impacts. The precursor impacts were found to be omitted in Dunn, et al. (2012b). A revised inventory for manganese carbonate was therefore compiled. Most manganese is currently produced in China; therefore, 20,000km by bulk commodity carrier was applied to account for shipping to Europe.

Manganese carbonate is suggested to be produced via leaching from manganese ores to form MnSO₄, followed by reactions with Na₂CO₃ to obtain MnCO₃ and Na₂SO₄ (Chow, et al. 2010; Glück, et al. 2012). To provide estimates for these operations, the Ecoinvent inventory for manganese concentrate was adapted to include the additional material flows for these steps, based on stoichiometric calculations, see Table 4.12.

Inputs	Amount	LCI data used	Notes
Manganese	1130 g	Ecoinvent dataset -	Used as proxy for 756g of MnO ₂
concentrate		manganese concentrate	base on required amount of Mn
		(42.4% Mn)	
SO ₂	557 g	Ecoinvent dataset -sulphur	Used for aqueous SO ₂ leaching
		dioxide, liquid	solution to obtain MnSO ₄
Na ₂ CO ₃	923 g	Soda	Sodium carbonate
Outputs			
MnCO ₃	1000 g		
Na ₂ SO ₄	1240 g	Ecoinvent - sodium	By-product, avoided burdens
		sulphate, powder	credit given
Waste	370 g	Ecoinvent - disposal, non-	Waste from manganese
		sulfidic tailings	concentrate

 Table 4.12 Modified inventory for manganese carbonate

Synthesis of the ultimate $LiMn_2O_4$ first involves ensuring that the precursors exhibit the correct size and shape to enable the desired properties. The Mn_2O_3 is then mixed with Li_2CO_3 and calcined at temperatures in the range of 600 to 900°C for 12 to 24 hours to produce $LiMn_2O_4$ (Iwata, et al. 2001; Cho, et al. 2012; Jung, et al. 2012).

Due to limited data, the inventory used was based on the Ecoinvent process for lithium manganese oxide. This included energy requirements of natural gas, 15.3MJ/kg and electricity, 0.005kWh/kg. These values were checked using the enthalpy of the reaction and heat required to raise the reactants temperature by 600°C, which gave a requirement of 2.61MJ per kg of LiMn₂O₄. However, this value does not account for any losses, maintaining the temperature, additional heat treatments or mixing and milling of the precursors (Iwata, et al. 2001; Cho, et al. 2012; Jung, et al. 2012). This suggests that the dataset may overestimate the heat (natural gas) and underestimate the electricity requirements. Therefore revised data should be sought as it becomes available.

Inventory for LFP cathode powder production

There are a number of different ways lithium iron phosphate powders can be synthesised (Jugović and Uskoković, 2009). The synthesis route modelled in this assessment is based on a patent from A123 Systems Inc. (Chiang, et al. 2012), who manufacture LFP batteries for EVs. The material inputs and outputs are given in Table 4.13 and were derived using stoichiometric calculations (Armand, et at. 2003; Chiang, et al. 2012).

The electrical energy required was based on the following processes:

- Milling of the input materials, approximately 1.3 litres for 24 hours, based on data for operation of a roller miller (Glen Creston, 2013).
- Heating in a tube furnace for 10 hours at 350°C and 20 hours at 600°C. The total energy used for this operation was estimated as 6.5MJ, based on that required to heat the reactants, vaporise the acetone and maintain the temperature using a 25KW tube furnace (Thermo Electron Corporation, 2005).

Inputs	Amount	LCI data used	Notes
Li ₂ CO ₃	234 g	See inventory for LMO cathode	
Iron (II)	912 g	Estimated using stoichiometric	No process
oxalate		calculations and precursors of	requirements included,
(FeC_2O_4)		acetic acid and Ecoinvent - iron	therefore may
		sulphate	underestimate impacts
Ammonium	729 g	Modified Ecoinvent -	Adapted to provide
phosphate		monoammonium phosphate	proxy for ammonium
$(NH_4H_2PO_4)$			phosphate
Acetone	206 g	Acetone	(DOE, 2010c)
Electricity	20.9MJ	Default data	14.4MJ milling, 6.5MJ
			heating
Outputs			
LiFePO ₄	1000 g		
CO ₂	558 g	Flow - Carbon dioxide [Inorganic	
		emissions to air]	
H ₂ O	171 g	Flow - Water vapour [Inorganic	
		emissions to air]	
Ammonia	5 g	Flow - Ammonia [Inorganic	95% efficient ammonia
(NH ₃)		emissions to air]	scrubbers assumed
			(DOE, 2010c)
Waste	326 g	Landfill for inert matter	Carbon and recovered
			emissions
Acetone	21 g	Flow - Acetone (dimethylcetone)	90% recovery assumed
		[to air]	(DOE, 2010c)
Waste heat	6.5MJ		

Table 4.13 Inventory for the production of LiFePO₄

Inventory for NCM cathode powder production

The performance of NCM is severely affected by the synthesis conditions and many different techniques have been proposed (Pan, et al. 2013). In this assessment the coprecipitation method has been modelled, because it was suggested to be suitable for large scale production and achieve the most controllable results (Wu, et al. 2012). This method involves producing a precursor material, in this case $Ni_xMn_yCo_{1-x-y}(OH)_2$, via precipitation processes, followed by reactions with Li_2CO_3 . The ratios of the materials in NCM also vary. For consistency, the ratios used were based on the composition $Li_{1.05}(Ni_{4/9} \text{ Mn}_{4/9} \text{ Co}_{1/9})_{0.95}O_2$, which was used to derive the cell performances/masses, see Section 4.3.5.

 $Ni_xMn_yCo_{1-x-y}(OH)_2$ was assumed to be prepared by reacting aqueous solutions of NiSO₄, CoSO₄, and MnSO₄ with NaOH. This involves heating the solution to around 50-60°C and stirring for around 12 hours (Lee, et al. 2004; Huang, et al. 2012). The amounts of the precursors required were based on stoichiometric calculations, see equation (4.2).

$$4/9NiSO_4 + 1/9CoSO_4 + 4/9MnSO_4 + 2NaOH \rightarrow Ni_{4/9}Mn_{4/9}Co_{1/9}(OH)_2 + Na_2SO_4$$
(4.2)

Due to a lack of data on the metal sulphates, they were approximated using datasets for pure metals. Improved data is also needed on the losses, additional processing materials and energy requirements. The inventory used is given in Table 4.14.

Inputs	Amount	LCI data used	Notes
Nickel	287 g	Nickel mix	Used as proxy for 756g of NiSO ₄
Cobalt	72 g	Ecoinvent – cobalt	Used as proxy for 189g of CoSO ₄
Manganese	268 g	Ecoinvent –	Used as proxy for 736g of MnSO ₄ , old
		manganese	dataset references 1994
NaOH	878 g	Sodium hydroxide	
Water	70 litres		Estimated for 2 mole/l solutions of input
			materials (Lee, et al. 2004)
Electricity	25.2 MJ	Default data, see	Estimate for mixing ≈3kWh (INDCO
		Section 4.3.5	Inc, 2013) and energy to heat solution,
			using specific heat of water and losses
Outputs			
Ni _{4/9} Mn _{4/9}	1000 g		
Co _{1/9} (OH) ₂			
Na ₂ SO ₄	1558 g	Ecoinvent - sodium	By-product, avoided burdens credit
		sulphate, powder	given
Water	70 litres	Waste water	Slightly organic and inorganic
		treatment	contaminated
Waste heat	14.4 MJ		

Table 4.14 Inventory for NCM precursor material production

The modelled final NCM synthesis involved heating the Ni_{4/9} $Mn_{4/9}$ Co_{1/9}(OH)₂ with Li₂CO₃ at around 950°C for 16h (Lee, et al. 2004; Huang, et al. 2012). The inventory use for this process is given in Table 4.15, based on stoichiometric calculations and assuming water/CO₂ as the by-products. The energy requirement was estimated using an approximate specific heat capacity of 1kJ/kg K, plus additions for maintaining the temperature and losses (Carbolite, 2013).

Material inputs	Amount	LCI data used	Notes
Li ₂ CO ₃	444 g	See inventory for LMO	7% excess (Huang,
		cathode	et al. 2012)
$Ni_{4/9} Mn_{4/9} Co_{1/9} (OH)_2$	925 g	See Table 4.14	
O ₂	90 g	Flow - Oxygen [Renewable	
		resources]	
Electricity	4.3MJ	Default data	Estimated
Outputs			
Li1.05(Ni4/9 Mn4/9	1000 g		
Co _{1/9}) _{0.95} O ₂			
CO ₂	247 g	Flow - Carbon dioxide	
		[Inorganic emissions to air]	
H ₂ O	183 g	Flow - Water vapour	
		[Inorganic emissions to air]	
Waste	29 g	Landfill for inert matter	Excess Li ₂ CO ₃
Waste heat	4.3 MJ		

Table 4.15 Inventory for NCM production

4.4.5. Separator

Microporous polyolefin membranes are widely used for the separators of lithium-ion batteries and are typically constructed of polyethylene or polypropylene, or layers of these materials. Two methods can be used to manufacture these separators termed wet and dry. The dry method was selected for this assessment because it is expected to be extensively used for the separators in future EV batteries and the process itself should not release any emissions (Baldwin, 2009; Mitsubishi Chemical Holdings Corporation, 2011).

This manufacturing technique involves melting and extruding (blow process) the base materials (polyolefin resin) into films at around 190°C, followed by thermal annealing and stretching to give the required microporous structure (Arora and Zhang, 2004; Funaoka, et al. 2011).

Little data on these operations could be found, but the majority of the separator cost is known to result from the material processing. For example, the input materials cost under $\pm 1/kg$, whereas the final separator costs more than $\pm 80/kg$ and optimistic long term values are still around $\pm 26/kg$ (Gaines and Cuenca, 2000; MTI Corporation, 2013a). This suggests significant processing is involved during their manufacturing.

To provide an estimate for the production processes the following methodology was used. An electrical energy requirement of 7.2MJ/kg was employed to account for the extrusion of the inputted polyethylene granules into an initial film. This value was based on the data for extrusion processes which typically have an energy consumption of 1.8 to 7.2MJ/kg (Mersiowsky, 2012), using the higher end of the scale to account for the specialist output being produced.

This value was used as a proxy for the subsequent two processes, adding a further 14.4MJ/kg, because although they differ from the extrusion process they also consist of heating and mechanical manipulation. A loss of 8% was applied to account for the processing yields (Yu, 2003) and a further 8% to allow for trimming of the separator, based on that for the electrode substrates (see Section 4.4.3). The inventory is given in Table 4.16.

Inputs	Amount	LCI data used	
Polyethylene	1180 g	Plastics Europe dataset available via GaBi	
		Polyethylene high density granulate (PE-HD)	
Electricity	21.6 MJ	Default data	
Outputs			
Separator	1000 g		
Waste	180 g	Granulation process modelled and credit given to	
		output for avoided burdens of polyethylene	
Waste heat	15.8 MJ		

Table 4.16 Inventory for separator production

4.4.6. Electrolyte

The electrolytes of lithium-ion batteries commonly consist of lithium hexafluorophosphate (LiPF₆) in a blend of solvents such as ethylene carbonate, dimethyl carbonate, diethyl carbonate and ethylmethyl carbonate. All tend to contain ethylene carbonate and concentrations of $LiPF_6$ are typically 1 mole per litre (Kawamura, et al. 2006).

In this assessment ethylene carbonate was used as the solvent, which for a 1 mole solution, gave a mass ratio of approximately 0.12 LiPF_6 to 0.88 ethylene carbonate. The impacts of producing the electrolyte were based on data from DOE (2010d) and stoichiometric calculations were used for the required precursors. The inventory is given in Table 4.17 and further details on LiPF₆ production are provided in the following subsection.

The specific operations included in this step were purification of the liquid solvents, blending of the constituents and packing. The amounts of some of the emissions are minimal, but they have been included for completeness.

Inputs	Amount	LCI data used	
Ethylene	967 g	Ecoinvent- CN: ethylene carbonate, with additional	
carbonate		transportation from China to Europe	
LiPF ₆	132 g	See following subsection	
Water	3.6 litres	Flow - Water (well water)	
Electricity	6.3 MJ	Default data	
Outputs			
Electrolyte	1000 g		
Waste water	3.6 litres	Assumed to be treated onsite	
Waste (landfill)	40 g	Landfill (Commercial waste for municipal disposal)	
Hazardous waste	11.6 g	Treatment of sludge (hazardous low level)	
СО	0.11 g	Flow - Carbon monoxide [Inorganic emissions to air]	
NOx	0.04 g	Flow - Nitrogen oxides [Inorganic emissions to air]	
SO ₂	0.001 g	Flow - Sulphur dioxide [Inorganic emissions to air]	
VOC	0.19 g	Flow - VOC (unspecified) [Organic emissions to air]	
PM _{2.5}	0.011 g	Flow - Dust (PM2.5) [Particles to air]	
PM ₁₀	0.011 g	Flow - Dust (PM2,5 - PM10) [Particles to air]	
CO ₂	156 g	Flow - Carbon dioxide [Inorganic emissions to air]	

Table 4.17 Inventory for electrolyte manufacture

Data on the process efficiency was unavailable. Therefore it was calculated assuming that the wastes and carbon content of the CO_2 resulted from lost input materials (the masses of the other emissions were deemed negligible). This gave an efficiency of approximately 91%.

Lithium hexafluorophosphate manufacture

Data on the production of LiPF₆ is very limited which has led to various methodologies being employed in existing battery LCAs. For example, Dunn, et al. (2012b) includes an energy value for the synthesis of LiPF₆ but did not consider the impacts of the precursors; Majeau-Bettez, et al. (2011) used generic inorganic chemicals as a proxy and assumed negligible additional energy requirements; and Notter, et al. (2010) derived values based on patents, estimates and stoichiometric calculations. These differing methodologies and assumptions have resulted in large variations between the production impacts. Therefore, a separate review was conducted to generate a new inventory. Safety must also be appreciated when dealing with LiPF₆ because it decomposes, if exposed to water, forming hydrofluoric acid which is extremely hazardous (Kawamura, et al. 2006).

Lithium hexafluorophosphate (LiPF₆) is commonly prepared by reacting phosphorus pentafluoride (PF₅) and lithium fluoride (LiF). Various processes and precursors can be used to prepare PF₅ (Liu, et al. 2010; Luly, et al. 2010). The data used in this assessment was based on details for a proposed new large scale manufacturing plant and patents by Honeywell, for which some information on emissions was available (Luly, et al. 2010; DOE, 2010e). These sources synthesise PF₅ by feeding streams of phosphorus vapour or liquid, and fluorine vapour into a reactor, usually at temperatures above 200°C, see equation (4.3).

$$P + 2.5F_2 \rightarrow PF_5 \tag{4.3}$$

The produced PF_5 gas is then circulated through a solution of hydrogen fluoride containing LiF to produce LiPF₆, which is collected by evaporating the hydrogen fluoride. The inventory approximated is given in Table 4.18 and was assumed to include the impacts of natural gas used during the processing. An efficiency of 94% was calculated from the emissions of LiPF₆ and stated control device effectiveness of 95% (DOE, 2010e). This was used together with stoichiometric calculations to approximate the required precursors. The hydrogen fluoride consumption was calculated in a similar manner.

Material inputs	Amount	LCI data used	
Fluorine	665 g	Ecoinvent - Fluorine [unspecified]	
Phosphorus	217 g	Ecoinvent - Phosphorus [industrial]	
Lithium fluoride	182 g	Ecoinvent - Lithium fluoride. Modified to incorporate	
		new Li ₂ CO ₃ inventory given in Section 4.4.4	
Hydrogen fluoride	30 g	Hydrogen fluoride	
Water	5.2 litres	Flow- Water (well water)	
Electricity	13.8 MJ	Default data	
Outputs			
LiPF ₆	1000 g		
Water	5.2 litres	Assumed to be treated onsite	
CO ₂	483 g	Flow - Carbon dioxide [Inorganic emissions to air]	
Hazardous waste	90 g	Treatment of sludge (hazardous low level)	
СО	0.3 g	Flow - Carbon monoxide [Inorganic emissions to air]	
PM ₁₀	1.9 g	Flow - Dust (PM10) [Particles to air]	
Fluorine	0.01 g	Flow - Fluorine [Inorganic emissions to air]	
Hydrogen fluoride	2.4 g	Flow - Hydrogen fluoride [Inorganic emissions to air]	
Nitrogen oxides	0.2 g	Flow - Nitrogen oxides [Inorganic emissions to air]	
Phosphorus	0.06 g	Flow - Phosphorus [Inorganic emissions to air]	
Sulphur dioxide	0.02 g	Flow - Sulphur dioxide [Inorganic emissions to air]	

Table 4.18 Inventory for LiPF₆ production

Several other emissions were also suggested to result from the manufacturing plant for which no characterisation flows were available. These were assumed to have minimal effects due to their very low quantities, with the exceptions of PF_5 and $LiPF_6$. These are known to decompose with moisture to form hydrogen fluoride (Kawamura, et al. 2006). Therefore, to account for some of their impacts, additional hydrogen fluoride emissions were applied based on stoichiometric calculations.

4.4.7. Cell casing and electrode terminal production

Several different casing options and materials are used for lithium-ion cells, e.g. stainless steel cylindrical cans, plastic prismatic cases and laminated pouches. In this assessment heat-sealable laminated aluminium pouches have been used because they are cheap, lightweight, commonly used in BEVs and mimic the type assumed during the derivation of the cell masses in Table 4.3 (AESC, 2013).

To produce the cell containers the material is formed into cell halves which are sealed together encapsulating the cell innards. Forming of the casing halves was modelled using process data for aluminium drawing, including a 20% loss. The constituents of the laminated pouch material were calculated based on data from MTI Corporation (2013b).

The inventories for the cell casing and electrode terminals are given in Table 4.19 and Table 4.20 respectively. A 5% loss was used to account for trimming during the production of the cathode and anode terminals.

Inputs	Amount	LCI data used	Notes
Aluminium foil 40µm	721 g	Aluminium foil	
Polypropylene (PP)	241 g	Polypropylene Film (PP)	
40µm		without additives	
Polyamide 25µm	191 g	Polyamide 6 Granulate (PA	Process dataset for
		6)	"Plastic Film" added
Adhesive	47 g	Polyester resin unsaturated	Used as proxy
Electricity	3.2 MJ	Default data	For "Aluminium
			sheet deep drawing"
Outputs			
Cell container	1000 g		
Waste Polyamide	32 g	Polyamide incineration	Laminate waste from
			drawing
Waste PP and	48 g	Waste incineration of	Laminate waste from
adhesive		plastics (PE, PP, PS, PB)	drawing
Waste aluminium	120 g	Aluminium foil scrap credit	

Table 4.19 Inventory for cell casing production

Inputs	Amount	LCI data used
Aluminium foil	245 g	Aluminium sheet
Copper foil	808 g	Copper mix from electrolysis
Outputs		
Cell terminals	1000 g	
Waste aluminium	12 g	Aluminium foil - scrap credit given using ingot mix
Waste copper	40 g	Credit for recycling, see note in Section 4.4.3.

Table 4.20 Inventory for cell terminal production

4.4.8. Final cell assembly

Final assembly of the cell has been taken to include attachment of the electrode tabs and sealing of the contents into the cell pouches. Other operations, e.g. sizing of the electrodes, have been incorporated in the previous sections.

Due to the hazards associated with LiPF_6 (see Section 4.4.6), operations where the electrolyte is exposed, i.e. filling the cell and sealing the case, have to be performed in dry rooms. These are suggested to consume significant amounts of energy (Smith, 1996; Dunn, et al. 2012b). Dry room requirements depend on many factors including the size, any occupant moisture, door openings, the external climate and cell throughput (Smith, 1996).

The dry room requirements were approximated from data given in Dunn, et al. (2012b). This data was verified using a dry room requirement of $4m^2$ /MWh per annum, for lithiumion battery manufacturing, calculated from Simon (2012), and energy consumptions from Smith (1996). This gave requirements of 0.29kWh of electricity and 1.9MJ of natural gas per kg of cell produced, which are similar to those of Dunn, et al. (2012b).

Additional energy requirements to maintain clean rooms (fans, filters etc.), stack the electrodes and inject the electrolyte (Reinhart, et al. 2012), were anticipated to be small compared to the dry room requirements and therefore omitted. Venting of the cell to remove gases generated during the formation cycle may also be necessary followed by further final cell sealing (Mikolajczak, et al. 2011; Kendrick, 2013). No suitable data could be found regarding the impacts of these operations and further work is thus needed to quantify them.

The electrode tabs were assumed to be connected to the electrode foils by ultrasonic welding (Nelson, et al. 2011b). The requirements were based on machine data from Branson (2011). Data for a laminated aluminium pouch sealer (MTI Corporation, 2013c) was used to estimate the cell sealing impacts. The inventory derived is given in Table 4.21.

Inputs	Amount	LCI data used	Notes
Compressed	6 litres	Compressed air – 7	Used by welding and sealing
air		bar	machinery
Electricity	0.8 MJ	Default data	0.7MJ dry room, 0.1MJ rest
Natural gas	1.3MJ	Default data	Dry room requirement

Table 4.21 Inventory for cell assembly

4.4.9. Cell formation and testing cycles

A "formation" cycle is required for new lithium-ion cells, during which reactions take place at the interface between the anode and electrolyte (Vettera, et al. 2005). This results in the formation of a protective layer on the surface, called the solid electrolyte interphase, which helps prevent any further reactions with the electrolyte while still permitting lithium ions to flow. This layer consumes lithium which results in irreversible capacity loss. Typical efficiencies for the formation cycle are around 80% to 90% (Wolter, et al. 2012). For this assessment an average value of 85% was used.

Along with the formation cycle, further tests are needed to verify the cells quality (Wolter, et al. 2012). These were modelled as one complete charge and discharge cycle. The energy efficiency of the batteries (see Section 2.3.2) for this step was taken as 94% and split equally between the charge/discharge cycles, to provide a simple estimation, giving 97% for each (Kuhn, et al. 2005).

During the formation and testing cycles the monitoring equipment and chargers/ dischargers used will also consume energy. To account for these requirements an efficiency of 90% has been used (Campanari, et al. 2009). Equations (4.4) and (4.5) show the calculations used to derive the energy consumptions for the formation and testing cycles. These gave a total energy requirement of 2.7 MJ/kWh which was converted to a mass basis using the cell specific energy and added to the electricity requirements used during final cell assembly in Table 4.21.

Electricity consumed during formation cycle:

Formation cycle energy (kWh/kWh of cell capacity) = $[1/(\eta_{fc}*\eta_{ee}*\eta_c)] - (1*\eta_c*\eta_{ee})$ (4.4)

Electricity consumed during test cycle:

Test cycle energy (kWh/kWh of cell capacity) = $[1/(\eta_{ee} * \eta_c)] - (1*\eta_c*\eta_{ee})$ (4.5)

Where:

 η_{fc} = Formation cycle efficiency

 η_{ee} = Battery energy efficiency

 $\eta_c = Charger/discharger$ efficiency

4.4.10. Battery pack non-cell components

In this section the inventories for the non-cell components in Table 4.2 are discussed.

Module production

The individual cells are grouped into modules. The additional components used to construct the modules have been taken as an aluminium housing, plastics supports/separators, and copper terminals (Table 4.2). The inventories for each of the components are given in Tables 4.22 to 4.24. Modules also often contain sensors and slave BMS circuit boards, however these components have been grouped under the separate BMS and wiring values (Ikezoe, et al. 2012).

Inputs	Amount	LCI data used
Aluminium sheet	1500g	Aluminium ingot mix
Process for - Aluminium sheet	1500 g	Aluminium sheet deep drawing (using
drawing		dataset default loss)
Electricity used for "Aluminium	3.2 MJ	Default data
sheet deep drawing"		
Outputs		
Module - casings	1000 g	
Waste aluminium	500 g	Aluminium foil - scrap credit given
		using aluminium ingot mix burdens

Table 4.22 Inventory for module casings

Inputs	Amount	LCI data used
Polypropylene	1020g	Polypropylene granulate (PP) mix
Process for - Plastic	1020 g	Plastic injection moulding part (unspecific)
injection moulding		
Outputs		
Module -	1000 g	
insulation/supports		
Waste polypropylene	20 g	Landfill (Commercial waste for municipal
		disposal)

Table 4.23 Inventory for module insulation/supports

Inputs	Amount	LCI data used
Copper	1230g	Copper mix (from electrolysis)
Process for - copper	1230 g	Ecoinvent - copper product manufacturing,
product manufacturing		average metal working
Outputs		
Module – terminals	1000 g	
Waste copper	230 g	Credit for recycling

Table 4.24 Inventory for module terminal production

Battery management system

Battery management systems (BMS) are a vital part of EV lithium-ion battery packs and have been identified as a substantial contributor to the production impacts (see Section 3.4.1). They are necessary to help optimise the pack performance and life, balance the cells and prevent hazardous or damaging situations from occurring.

To monitor and help prevent such situations, BMS can incorporate a variety of components. For example:

- Temperature sensors
- Pressure sensors
- Voltage sensors
- Control circuits
- Relays, shunt resistors, cut-offs, fuses and disconnects
- And all the necessary wiring and connectors.

No specific data for BMS circuit boards was available. Therefore generic processes available from Ecoinvent were assessed for their suitability. Initially the Ecoinvent process *,printed wiring board, surface mounted, unspec., Pb free*" was selected as a potentially suitable proxy (Ecoinvent, 2012). This process has high impacts, 251kg of CO_{2e} emissions per kg. Review of the process revealed the majority of this impact, 175kg CO_{2e}, resulted from a 0.173kg input of the feed process *,integrated circuit, IC, logic type*", which has extremely high impacts, e.g. 1010kg CO_{2e} and 15500MJ of primary energy per kg. Compared to data from studies of computer integrated circuits, for which ranges of 160 to 700kg CO_{2e} and 2100 to 8100MJ of primary energy per kg have been reported (Teehan and Kandlikar 2012), these values appear high. New estimates of the integrated circuit mass

contained on a BMS board were made, using a board from a LiFeBATT 2E-108015 108V/15Ah battery pack (see Figure 4.6). This indicated the integrated circuit represented approximately 2% of the mass, which is far lower than the 17.3% used in the generic Ecoinvent process. Considering the already high integrated circuit impacts, this is likely to result in the Ecoinvent circuit board inventory estimating substantially higher impacts than those associated with BMS boards.



Figure 4.6 BMS circuit board

To provide a more representative value the Ecoinvent process was adapted, based on the estimates from the LiFeBATT BMS, to give the inventory shown in Table 4.25. The changes made were to decrease the mass of the integrated circuits and base board, and to increase the resistor and connector masses. The Ecoinvent process for integrated circuits is still employed, however the far lower input mass should minimise its impacts.

Table 4.26 gives the inventory used for the other BMS components (relays, sensors, fuses etc.) shown in Table 4.2, which were approximated as consisting of high power relays, 80%, and connecters, 20%. The BMS wiring was based on the same inventory as the main cabling see following section.

Ecoinvent input process	Quantity	Unit
Capacitor, SMD type, surface-mounting, at plant	0.033	kg
Connector, PCI bus, at plant	0.06	kg
Diode, glass-, SMD type, surface mounting, at plant	0.004	kg
Disposal, treatment of printed wiring boards [Recycling]	0.020	kg
Integrated circuit, IC, logic type, at plant	0.022	kg
Light emitting diode, LED, at plant	0.001	kg
Mounting, surface mount technology, Pb-free solder	0.21	sqm
Printed wiring board, surface mount, lead-free surface, at plant	0.21	sqm
Resistor, SMD type, surface mounting, at plant	0.245	kg
Transistor, SMD type, surface mounting, at plant	0.010	kg
Transport, transoceanic freight ship	0.806	tkm
Transport, freight, rail	0.143	tkm
Transport, lorry >16t, fleet average	0.133	tkm

Table 4.25 Inventory used to model the BMS circuit boards

Inputs	Amount	LCI data used	Notes
Relays	800 g	Ecoinvent - transformer,	Transformers used as proxy for
		high voltage use	relays which contain similar main
			components i.e. plastic housings,
			coils and connectors
Connectors	200 g	Ecoinvent - connector,	
		PCI bus, at plant	
Outputs			
BMS	1000 g		BMS components excluding
			wiring and circuit boards

Table 4.26 BMS inventory excluding wiring and circuit boards

Main cabling and BMS wiring

The cabling was assumed to consist of 66% copper and 34% polyvinyl chloride (PVC) by mass, based on the percentages used in the Ecoinvent process for cable EoL treatment. These values were verified against data for insulated single core cables used in vehicles (AES, 2014).

The inventory is presented in Table 4.27 and was based around the Ecoinvent process "single core conductor cable", but with modifications to the input materials. A 2% loss for trimming and fitting of the connectors was included.

Inputs	Amount	LCI data used
Copper	673 g	Copper mix (from electrolysis)
Wire drawing	673 g	Copper wire (0.6 mm)
PVC	347 g	Polyvinylchloride granulate (Suspension, S-PVC)
Plastic extrusion	347 g	Plastic extrusion profile
Transport	0.204 tkm	Ecoinvent - transport, freight, rail
Transport	0.102 tkm	Ecoinvent - transport, lorry >16t, fleet average
Outputs		
Cabling	1000 g	
Waste cable	20 g	Ecoinvent- treatment, cable - with credit for
		copper recycling and incineration of PVC

Table 4.27 Inventory for cabling

Other non-cell components

The remaining components listed in Table 4.2 were modelled as shown in Table 4.28.

Component	LCI data used	Processing modelled	Loss and waste treatment
Bus bars	Copper mix (from	Sheet stamping based	10% loss with recycling
and	electrolysis)	on data for steel sheet	credit given for copper
terminals		stamping/bending	
Pack plastic	Polyvinylchloride	Plastic injection	2% loss, municipal disposal
- PVC	granulate	moulding (unspecific)	
Pack plastic	Polypropylene	Plastic injection	2% loss, municipal disposal
- PP	granulate mix	moulding (unspecific)	
Pack (steel)	Steel cold rolled	Steel sheet stamping	5% loss with credit for steel
	coil	and bending	recycling
Fixings	Stainless steel	Punching steel sheet	56% loss according to
	cold rolled coil	small part	process, recycling credit
	(316)		given

 Table 4.28 Data used to model remaining pack components

In addition to the processes shown, the steel proportion of the pack casing was assumed to be powder coated for protection using the Ecoinvent process for "powder coating, steel". The plastic proportion of the casing was split by mass into polypropylene 80%, for the case/module supports, and PVC 20%, for the insulating covers/seals (VTE Europe, 2013).

The components shown contain only single materials, therefore the required input amounts per unit mass were one plus the percentage losses shown.

4.4.11. Final battery pack assembly

Assembly of the battery has been taken to include construction of the modules followed by fitment of the modules, BMS and wiring into the battery case and finally sealing of the case. The component manufacturing processes, e.g. forming of the casing, were incorporated in the relevant production inventories. Table 4.29 shows the process inventory used per kg of final battery pack produced.

Inputs	Amount	LCI data used	Notes
Laser	0.3m	Aluminium laser welding (1 to	Attachment of the module
welding		3.5mm depth). Used as proxy for	terminals (Nelson, et al.
		copper welding	2011b)
Crimping	0.05 kg	Process for ,Steel sheet stamping	Joining of module housing
		and bending", used as proxy	
		with no losses	
Compressed	20 litres	Compressed air 7 bar	Estimate for air used by
air			assembly ratchets etc.
Electricity	0.11MJ	Default data	Estimate for conveyer
			belts and assembly robots

Table 4.29 Data used to model battery pack assembly

4.5. Battery pack end-of-life inventory

This section details the methodology, assumptions and data sources used to model the battery pack end-of-life. Some of the raw data used was confidential, which precluded the reproduction of particular values. This was however primary data taken from trials of EV battery pack recycling processes and should help improve the quality of the results.

The operations modelled are based on a hydrometallurgical route as discussed in Section 2.3.2 and the process diagram is shown in Figure 4.7.



Figure 4.7 Process diagram for battery pack recycling

4.5.1. Battery pack removal

The first step in the battery recycling process is to remove it from the vehicle. Following removal, the rest of a BEV is suggested to be treated in a similar manner to a conventional vehicle (BIS, 2011).

Much of the work involved in the above step is anticipated to be performed by hand. However, there will be small amounts of electricity and compressed air required to operate ramps, ratchets and the remainder of the facility. To provide a proxy for these values, the same requirements as found for battery pack assembly were used, see Table 4.29.

4.5.2. Dismantling and discharging of the battery pack

The extent to which the pack is dismantled will depend upon the particular pack, economics, recycling targets and subsequent processes used. For consistency with the production inventory, the battery pack in this assessment was assumed to be dismantled into the components listed in Table 4.2. At present this operation is very labour intensive, but in the future more automated dismantling may be used to reduce processing costs.

Confidential values were used to model the requirements of these operations.

4.5.3. End-of-life treatment of non-cell components

The non-cell battery pack components, obtained during the dismantling phase, were assumed to be treated in the same manner as general wastes of the same materials. The specific processes modelled are given in Table 4.30. The polypropylene and PVC components (i.e. plastic pack and module insulation/supports) were modelled as being directly recycled, because the dismantling process should yield significant streams of unmixed plastics (Al-Salem, et al. 2009).

Component	Material	Process used for waste treatment
Bus bars and	Copper	Recycling credit applied
module terminals		
Pack (plastic) and	Polypropylene	Reprocessing modelled using processes for
module insulation		washing, granulating and compounding/
/ supports		pelletizing. Credit given (excluding losses), for
		substituted primary polypropylene granulate.
Pack (plastic)	PVC	Reprocessing using processes for washing,
		granulating and compounding/pelletizing. Credit
		given for substitution of PVC granulate.
Pack (steel)	Steel sheet	Recycling credit applied (GaBi value for scrap)
Fixings	Stainless steel	Recycling credit applied (GaBi value for scrap)
Main cabling and	PVC coated	Ecoinvent process for "mechanical separation of
BMS wiring	copper	copper containing cables". Outputs treated by
		applying copper recycling credit and incineration
		with electricity generation for the PVC.
BMS (circuit	Circuit board	Ecoinvent process "Populated printed wiring board
boards only)		incineration" with credits for electricity
		generation.
BMS (relays,	80% relays	Ecoinvnet process for "mechanical treatment,
sensors, fuses	20%	industrial devices" used as proxy. Credits applied
etc.)	connectors	for outputs of copper, aluminium and steel.
Module casing	Aluminium	"Aluminium foil - scrap credit" used with credits
	sheet	given for substituted aluminium ingot mix.

Table 4.30 Processes used to model EoL treatments of non-cell components

4.5.4. Cell recycling

The first step in the cell recycling process is crushing in an inert atmosphere containing carbon dioxide. The inert atmosphere prevents safety hazards, e.g. sparks or explosions due to residual charge. The output is then sorted by sieving, magnetic separation and density segregation. These operations yield a magnetic fraction, high and low density non-magnetic fractions and a fine fraction rich in metal oxides and carbon (Tedjar and Foudraz, 2010). The requirements for these processes were based on confidential measurements.

The resulting output material streams were matched to the production inputs given in Table 4.3 and the model was parameterise to automatically compensate for the different cell chemistries. The treatments applied to the resulting materials are given in Table 4.31. Due to the relatively detailed processes involved with the cathode active materials and electrolyte, further descriptions of their treatments are given in the following subsections.

No specific data was available for graphite EoL treatment. Therefore impacts for incineration, with credits for electricity generation, were approximated using stoichiometric calculations and assuming the process converted all the material to CO_2 . The electricity generation credit was calculated based on the energy density of carbon, 32.8MJ/kg, and a plant efficiency of 30%. This route was found to result in large net CO_2 emissions due to the process being more carbon intensive than the electricity grid mix, EU average, it was assumed to displace. Therefore the model was parameterised to allow for a scenario where the graphite was instead sent to landfill.

Component	Material	Process waste treatment
Cathode electrode	Aluminium	GaBi scrap credit for aluminium foil
foil and terminal		applied
Anode electrode foil	Copper	Recycling credit given
and terminal		
Anode electrode	Graphite	Incineration with electricity generation
material		credit, see note in text
Cathode electrode	Active material	See following subsection
material		
Cathode carbon	Carbon	Processed with graphite, see above
Electrode material	Binder - styrene	Ecoinvent "disposal, rubber, unspecified,
binder	butadiene rubber	0% water, to municipal incineration"
Cell container	Laminated	"Aluminium foil - scrap credit" with credits
	aluminium	given for aluminium ingot mix. Plastic
		fraction modelled as being incinerated.
Separator	Polyethylene	Process for "Waste incineration of plastics
		(PE, PP, PS, PB)" with electricity credit
Electrolyte	Ethylene carbonate	See subsection below
	and LiPF ₆	

 Table 4.31 End-of-life treatments for cell materials

Cathode material recycling

There are numerous processes suggested for the recovery of metals from the fine fraction, obtained from the cell crushing processes, which offer different recovery efficiencies, purities and outputs (Lupi, et al. 2005; Xu, et al. 2008; Buchert, et al. 2011; Georgi-Maschler, et al. 2012; Granata, et al. 2012). For example, some processes may recover highly pure base metals, while others may recover them in the form of carbonates or sulphates. These may be suitable forms for their reuse but require less EoL processing.

In this assessment the outputs from recycling were selected to match the forms used during production as much as possible. This enabled credits for the avoided burdens to be applied that were consistent with the impacts incurred during the initial production. The specific material forms reclaimed were:

- Cobalt and nickel as pure metals.
- Manganese as manganese carbonate (Tedjar, F., 2004; Granata, et al. 2012).
- Lithium in the form of lithium carbonate.
- Due to the low values of iron and phosphorus, which are contained in LFP cathodes, they were modelled as being sent to landfill.

The recycling methodology used for the cathode active materials was modelled as follows. First leaching using a sulphuric acid solution at 80°C, was assumed (Tedjar and Foudraz, 2010). The energy required to heat the acid solution was estimated using the specific heat capacity of water for a temperature rise of 60°C. Significant mixing of the solution is also required (Mantuano, et al. 2006; Granata, et al. 2012), which was approximated as utilising 0.25kWh of electricity per kg.

Various possible extraction procedures are given in the literature (Mantuano, et al. 2006; Xu, et al. 2008). However details on the energy and materials consumed are limited. In this assessment electrolysis was assumed for the recovery of metallic cobalt and nickel (Lupi, et al. 2005; Tedjar and Foudraz, 2010). The energy requirements for this process were based on the results given in Lupi, et al. (2005), of 2.8 kWh/kg and 2.96 kWh/kg, for cobalt and nickel respectively. The recovery yields for this process are high, >95%, therefore no losses were incorporated in the model. The manganese and lithium were taken to be removed as carbonates via mixing with sodium carbonate (Tedjar, 2004). A process yield of 80% was used for lithium and all the manganese was assumed to be recovered (Granata, et al. 2012).

Table 4.32 presents the EoL inventory derived using stoichiometric calculations for the case of the $LiMn_2O_4$ cathode. Data for the other cathode materials was calculated in the same manner using the assumptions given above.

Inputs	Amount	LCI data used	Notes
Waste cathode	1000 g		Values for LiMn ₂ O ₄ presented
active material			
Water	13 kg	Water (deionised)	Calculated based on a 1 mol/l
(deionised)			sulphuric acid concentration
			(Tedjar and Foudraz, 2010)
Sulphuric acid	1350 g	Sulphuric acid mix	Based on stoichiometric
			quantities needed
Soda (sodium	1470 g	Soda (Na ₂ CO ₃)	Carbonate source
carbonate)			
Extractants	25 g	Chemicals inorganic	Proxy for chemicals used
			(Fisher, et al. 2006)
Heat from	3.55 MJ	Default data	Heating of the leaching
natural gas			solution
Electricity	0.9 MJ	Default data	Requirements for mixing and
			electrolysis of nickel/cobalt
Outputs			
Manganese	1270 g	Manganese carbonate -	Credit given for replacement of
carbonate		see Table 4.12	primary material
Lithium	164 g	See Section 4.4.4	Credit given for replacement of
carbonate			primary material, yield of 80%.
Sodium sulphate	1960 g	Ecoinvent -sodium	Credit given for sodium
		sulphate, powder,	sulphate (by-product from
		production mix	carbonate production)
Waste water	13 kg	Waste water treatment	
Waste	66g	Landfill for inert matter	Process wastes
		(Unspecific	
		construction waste)	
Waste heat	3.55 MJ		

Table 4.32 Recycling inventory for the active cathode material (LMO shown)

Recycling of the manganese content was found to result in increased impacts. This was due to the low values, associated with primary manganese carbonate production, being more than offset by those from the sodium carbonate and sulphuric acid used during its recycling. The model was therefore parameterised to allow for a scenario where the manganese is not reclaimed.

Electrolyte recycling

Limited data on EoL processing for the electrolyte was identified. Therefore the recovery was estimated based on a process patent which recovers lithium (in the form of lithium chloride), hexafluorophosphate and organic carbonate fractions (Pelgrims and Thijs, 2012).

The process first involves the substitution of the PF_6 - anion, from the LiPF₆ in the electrolyte, using an ionic liquid containing a chloride anion to form non-soluble LiCl which is collected by filtration.

The filtrate is then mixed with water to dissolve the organic carbonates (electrolyte solvents - ethylene carbonate in this assessment), leaving the ionic liquid containing the PF_6 , which is filtered out. The organic carbonates are then reclaimed by evaporating the water.

The resulting liquid containing the PF_6 - anions is suggested to have a commercial value above that of the input form containing the Cl^- anions. Therefore, to overcome a lack of data on these, it was assumed that the avoided burdens from the product liquid would offset those from the production of the input ionic liquid. They have subsequently been excluded from the inventory given in Table 4.33.

Inputs	Amount	LCI data used	Notes
Electrolyte	1000 g		Waste for recovery
Dichloromethane	1 g	Dichloromethane	Estimate for loss during
			washing of LiCl precipitate
Heat from	21.2 MJ	Default data	Estimate for heat to
natural gas			evaporate the water (base on
			heat of vaporisation) and dry
			the LiCl.
Water	7500 g	Water (deionised)	
Outputs			
LiCl	32 g	Ecoinvent - lithium	Credit for reclaimed material,
		chloride, at plant	using 95% recovery yield
			(Pelgrims and Thijs, 2012).
Ethylene	880 g	Ecoinvent- ethylene	Credit given for reclaimed
carbonate		carbonate	material.
Waste water	7500 g	Waste water treatment	
		(slightly organic and	
		inorganic contaminated)	
Waste	0.3 g	Landfill for inert matter	Unrecovered lithium
Dichloromethane	1 g	Flow - Dichloromethane	Fraction assumed not to be
		(methylene chloride)	recovered
		[emissions to air]	
Waste heat	21.2 MJ		

Table 4.33 Inventory for the recycling of the electrolyte

5. WHOLE LIFE VEHICLE MODEL

5.1. Methodology

This chapter describes the construction of the vehicle model, excluding the batteries, followed by the MATLAB[®] programme used to simulate the in-use phase and effects of key variables. These were subsequently combined with the battery life cycle inventory (LCI), developed in Chapter 4, to allow evaluation of the whole life cycle of a vehicle. Figure 5.1 shows the main components which constituted the whole model.

The vehicle LCI was constructed in two parts. The first compiled the inventory for the powertrain components of a battery electric vehicle (BEV), excluding the battery pack, and the second modelled a generic glider vehicle (complete vehicle excluding the powertrain). To provide a baseline to compare the BEV against, an inventory for the production of a conventional powertrain was also generated. This was combined with the glider vehicle LCI, to represent a complete conventional vehicle and GaBi/manufacturer data to model the use phase.

For consistency the scope was matched with that of the battery LCA given in Section 4.3 and therefore not repeated in this chapter. However, details are given for the functional unit and assessment boundaries which were adapted to encompass the whole vehicle.

The use-phase model details the vehicle parameters employed and the construction of the battery simulator. Existing LCAs have tended to provide limited evaluations of battery variables or only assessed them with respect to certain phases of a battery's lifetime (see Section 1.5 for further details). This model enabled the effects of battery parameters on the whole vehicle lifetime to be assessed and studies of the trade-offs between them to help identify optimal choices.

This is followed by validation of the model and a comparison of the result simulated over the New European Driving Cycle (NEDC) against real-world test data, see Figure 5.1.

The impacts calculated, effects of the parameterised variables and discussion of the main findings are provided in Chapter 7.



Figure 5.1 Main components of complete model

5.2. Assessment goals

The aim of the overall assessment was to help identify the effects of batteries on the whole life impacts of BEVs and how variations in some of their parameters can affect the results. This should enable optimal trade-offs to be identified between components/parameters, especially those resulting from their batteries, which can minimise the impacts of BEVs.

Along with the objectives of the battery model, see Section 4.2, this assessment aimed to:

- Quantify the impacts of the battery packs used in BEVs on their whole life.
- Identify the significance of different lithium-ion battery cathode materials on the whole life impacts of BEVs.
- Assess how variations in battery parameters (e.g. lifetime and energy efficiency) affect the whole life impacts of vehicles.
- Identify areas where data limitations or variations remain, which could potentially have a significant bearing on the overall results i.e. areas requiring further work.
- Generate a framework which can make more holistic sustainability assessments of BEVs.

5.3. Assessment scope

This section details the main adaptations to the scope, given for the battery LCA in Section 4.3, to encompass the whole vehicle.

5.3.1. Functional unit

The functional unit for the overall model was set as the impacts associated with travelling 1km in a "C" segment vehicle with a range of 175km (109 miles), measured over the NEDC (see Figure 5.2).



Figure 5.2 Velocity profile of New European Driving Cycle

The range of 175km was selected to coincide with that currently claimed by many BEV manufacturers and to help ensure practical battery pack masses.

A "C" segment (also referred to as lower medium or small family) has been taken as a vehicle representative of those classified as "small family" by Euro NCAP (Euro NCAP, 2013), such as the Volkswagen Golf and Peugeot 308.

To isolate the impacts resulting specifically from the factors being analysed, see discussion in Section 2.2, the non-powertrain factors were held constant. Specifically the assessment used values based around those of the fully electric Nissan Leaf, see Figure 5.3 and Section 5.8, to allow reliable comparisons with test data taken from this vehicle.

The specification of a range dictated the required mass of batteries and thus total vehicle mass, for each of the chemistries. This thereby allowed the effects of the battery parameters to be evaluated for the same level of utility to the end user, i.e. range.



Figure 5.3 Nissan Leaf electric 'C' Segment vehicle

A lifetime distance of 150,000km over the NEDC was used to model the use phase (see Section 3.3.1). These parameters were chosen to aid comparisons with many existing assessments (Volkswagen AG, 2008; Notter, et al. 2010; Renault, 2011) and a sensitivity analysis was performed to evaluate their effects.

5.3.2. Assessment boundaries

The LCI presented in the following sections, along with that for the battery, encapsulated the production, use and EoL impacts associated with a BEV, as shown in Figure 5.4.

The use phase specifically encompassed:

- Production of the in-use energy e.g. electricity. This was based on GaBi data which included production, transmission losses and the impacts associated with the provision of the primary feedstocks.
- The losses arising from the battery charger.
- The vehicle use requirements, which included the losses associated with the vehicle components, e.g. the batteries and motor.
- Vehicle maintenance, which was based on approximations for the production and EoL treatments of the parts consumed during the vehicle"s lifetime.

The production and EoL phases were in line with those described for the battery LCA in Section 4.3.2.


Figure 5.4 Processes considered in assessment

5.4. Powertrain production

This section details the inventories used to model the powertrain components for a BEV (excluding the battery) and a conventional vehicle.

5.4.1. Battery electric vehicle powertrain

The inventory for the BEV powertrain is given in Table 5.1 and includes the electric motor (wound rotor synchronous machine), gearbox (single speed), charger, invertor and cabling (mass values given refer to those in the final components i.e. excluding manufacturing losses). The material inputs were mainly based on data for the Renault Fluence Z.E., for which a detailed inventory was available (Renault, 2011). This is a "C" segment BEV in line with the assessment scope. Several different motor types, e.g. permanent magnet and induction, are used in current BEVs that will alter the inventory. The effects of these on

BEV lifetime impacts are anticipated to be small considering, many of the materials/ processes are similar between these types and previous findings which suggest the total powertrain CO_{2e} impacts, excluding the battery, represent <6% of the lifetime value (Notter, et al. 2010). However, comprehensive inventories for powertrains using these alternatives are needed to verify this.

Inputs	Mass (kg)	LCI data used	Processing data used
Steel sheet	11.5	Steel finished cold	Steel sheet stamping and
		rolled coil - worldsteel	bending (5% loss)
Steel	34.5	Steel plate -worldsteel	Steel turning
Stainless	1.86	Stainless steel cold	Punching steel sheet small part
steel		rolled coil (316)	(25% loss set)
Aluminium	35.08	Aluminium ingot mix	Aluminium die-cast part and
			Aluminium cast part machining
Copper	15.85	Copper mix (from	Copper wire (0.6 mm)
		electrolysis)	
Elastomers	0.61	Styrene-Butadiene	No losses modelled due to low
mix		Rubber (SBR) Mix	mass
Synthetic	1.83	Ethylene Propylene	No losses modelled
rubber		Diene Elastomer	
Glass fibre	0.87	Nylon 6.6 GF30	No losses modelled due to low
filled nylon		compound	mass
Nylon	2.09	Nylon 6.6 granulate	Polyamide 6.6 (PA 6.6) GF
			injection moulded part
Polybutylene	1.22	Polybutylene	Plastic injection moulding part
Terephthalate		Terephthalate Granulate	(unspecific)
Polymers mix	4.14	Polypropylene	Polypropylene granulate
		granulate	injection moulded part
Polyurethane	0.43	Polyurethane flexible	No losses modelled due to low
		foam	mass
Electronic	3.76	See Table 5.2	
components			
Outputs			
Powertrain	114		

 Table 5.1 BEV powertrain inventory

Manufacturing requirements were approximated using generic datasets, including average losses, for common processes that are likely to be used to produce the components. The metallic production scrap was taken to be directly recycled and credits were applied accordingly. To provide a proxy for 3kg of unclassified materials, a constitution of 50% polypropylene and 50% aluminium was used.

In the breakdown of the Renault system the electronic components were aggregated, giving a mass of 3.76kg. To provide suitable inputs this mass was proportioned based on approximations of the components contained in EV invertors and chargers, see Table 5.2 (Infineon, 2011; Rahman, et al. 2011). The circuit board mass was estimated as 0.5kg, based on the required area of those shown in Burress, (2012) and Rahman, et al. (2011).

Inputs	Mass (kg)	LCI data used
Circuit board	0.5	Approximated using dataset derived for
		BMS see Section 4.4.10
Transistors (power module	0.15	Ecoinvent - Transistor, wired, big size,
etc)		through-hole mounting
Copper (power module base	0.1	Copper mix (from electrolysis)
plate)		
Aluminium oxide (proxy for	1.05	Ecoinvent - aluminium oxide
remainder of power module)		
Cable	0.36	Approximated using dataset for main
		cabling and BMS wiring see Section 4.4.10
Capacitors	1.2	Ecoinvent - capacitor, film, through-hole
		mounting
Resistor	0.2	Ecoinvent - resistor, unspecified
Electrical connectors	0.2	Ecoinvent - connector, PCI bus
Outputs		
Electronic components	3.76	

Table 5.2 Breakdown of electronic components

5.4.2. Conventional powertrain

The LCI for the conventional powertrain was adapted from existing in-house models (Raugei, 2013). The resulting model had a total mass of 267kg, which included the engine, cooling system, transmission, fuel system and exhaust, but excluded the fuel and lead-acid battery (the lead-acid battery was incorporated in the glider vehicle).

The model was intended to be representative of a powertrain suitable for a "C" segment vehicle, but does not refer to any particular configuration.

5.5. Glider vehicle production

For the purpose of this assessment the vehicle mass, excluding the battery pack whose mass differences were incorporated, was assumed to remain constant. Secondary mass savings, or penalties, may be achieved due to changes in the battery pack mass (Lewis, et al. 2012). For example a lighter pack may enable downsizing of other components, which will amplify the mass savings. However, the secondary savings/penalties from changes in the battery mass were anticipated to be small for the scenarios assessed.

5.5.1. Battery electric vehicle glider

The powertrains of BEVs (without the batteries), are lighter than those of conventional vehicles (Renault, 2011). However their large additional battery packs typically result in a greater total vehicle mass. This may in turn necessitate additions to the glider vehicle in order to cope with the resulting higher forces.

Lightweight materials are being used to compensate for the additional mass of traction batteries, for example the carbon fibre body shell being used in the electric BMW i3 (Kingston, 2013). These alterations could be employed on vehicles with any powertrain to reduce the in-use impacts, see Section 2.2.1. Therefore, to help ensure consistency when making comparisons with existing powertrains, the BEV glider was assumed to be constructed using predominately steel as currently found in most conventional vehicles.

The constituents of the glider vehicle were based on existing literature values (Schweimer and Levin, 2000; Burnham, et al. 2006; Volkswagen AG, 2008; Notter, et al. 2010; Eckstein, et al. 2011). To account for the larger overall mass of a BEV an additional mass of steel, above that used for a lighter conventional vehicle, was incorporated to simulate uprated structural components. This resulted in the selection of 1100kg, for the glider

mass. Using the powertrain mass of 114kg (Table 5.1) and traction battery mass for a "C" segment vehicle of \approx 300kg (see Section 4.4.1), gave a vehicle mass of 1514kg, which was comparable to existing BEVs in this class e.g. the Nissan Leaf and Renault Fluence Z.E.

The glider was first broken-down into the components shown in Table 5.3 and then inventories for the materials used in each were compiled, see Table 5.4. The values shown do not represent any one particular vehicle and could vary significantly depending upon the design and material choices. However, due to traction batteries being the focus of this thesis, they were deemed sufficient to allow compilation of the whole vehicle model.

Component group	Mass (kg)	Main components in group
Steel body and chassis	725	Steel body structure, external panels, axels,
		brakes and suspension
Interior	160	Seats, insulation, door panels, dashboard and
		heating, ventilation and air-conditioning systems
Glass	40	Windows
Tyres	34	
Body hardware/fixings	30	50% steel 50% plastic
Exterior	26	Paint, trim/seals and lighting housings
Electrical	35	Wiring, motors, switches and circuits
Wheels	20	Aluminium
Lead-acid battery	16	Auxiliary battery
Fluids	14	Transmission oil, coolant, brake fluid and
		windscreen washer fluid

Table 5.3 Glider vehicle constituents

To account for manufacturing of the steel components a loss of one third was applied. This was modelled as being directly recycled (Renault, 2011). However, due to data limitations and their far lower masses, no losses were incorporated for the other glider materials.

The energy consumed during production was based on data from Volkswagen for a vehicle with a mass similar to that of the glider vehicle modelled (Schweimer and Levin, 2000). This gave requirements of 2140kWh of electricity and 7900MJ of heat from natural gas (used to approximate 2200MJ of natural gas and 5700MJ of heat energy), per glider vehicle. These were subsequently verified against data from Daimler, for their energy consumption and annual production, to ensure they were feasible (Daimler AG, 2013).

Component group	Inventory data and constituent percentages used	
Steel body and chassis	Steel finished cold rolled coil 100%	
Interior	Polypropylene granulate mix 25%	
	Polyurethane flexible foam 19%	
	Steel finished cold rolled coil 37%	
	Polyethylene high density granulate 6%	
	Aluminium ingot mix 3%	
	Aromatic Polyester Polyol 9%	
	Styrene-Butadiene Rubber mix 1%	
Glass	Float flat glass 100%	
Tyres	Ecoinvent - synthetic rubber 80%	
	Steel wire rod 20%	
Body hardware and	Polypropylene granulate mix 50%	
fixings	Steel finished cold rolled coil 50%	
Exterior	Alkyd paint 20%	
	Ecoinvent - synthetic rubber 38%	
	Polyvinylchloride granulate 42%	
Electrical	Cabling 43% based on battery cable data see Section 4.4.10	
	Circuit boards 6% based on BMS data see Section 4.4.10	
	Aluminium ingot mix 17%	
	Steel finished cold rolled coil 22%	
	Copper mix (from electrolysis) 12%	
Wheels	Aluminium ingot mix 100%	
Lead acid battery	Ecoinvent - lead, primary 69%	
	Water (deionised) 14%	
	Sulphuric acid (96%) 8%	
	Polypropylene granulate mix 7%	
	Glass fibres 2%	
Fluids	Ethylene glycol 22%	
	Process water 30%	
	Ecoinvent - Lubricating oil 32%	
	Ecoinvent - Refrigerant R134a 7%	
	Ecoinvent - Ethanol 9%	

Table 5.4 Data used to model glider vehicle

5.5.2. Conventional glider vehicle

To provide an approximation, for a comparative conventional vehicle glider, the same inventory used for the BEV was employed with a reduction in the steel content. This was to allow for lighter structural components due to the lower overall mass. This gave a total vehicle mass of 1317kg, including the powertrain (Section 5.4.2), which was comparable to existing ,,C^{**} segment vehicles such as the Ford Focus and Peugeot 308.

5.6. Maintenance

5.6.1. Battery electric vehicle

During the BEVs use phase, the lead-acid battery and fluids (with the exception of the windscreen washer fluid which was modelled as being renewed twelve times with the ethanol contained being released to the atmosphere) were assumed to require one replacement during the vehicles lifetime (Burnham, et al. 2006; Renault, 2011). The tyres were taken to require 4 replacements over the 150,000km lifetime and an input of 7.6kg of steel was applied to provide a proxy for maintenance of the braking system.

The same inventories employed in the initial glider vehicle were used to model these requirements.

5.6.2. Conventional vehicle

The maintenance of the conventional vehicle was based on that of the BEV, with the addition of 3kg of oil every 30,000km to account for periodic renewal of the engine oil.

5.7. End-of-Life

The EoL phase was modelled using a generic GaBi process for shredding/separation of a vehicle following depollution, with the material outputs adjusted to maintain consistency with those used in the manufacturing phase. Further EoL treatment of the reclaimed materials was approximated by applying the same assumptions as used for the battery model (see Section 4.3.5).

5.8. Use phase model

The BEVs use phase was modelled using a development of the MATLAB[®] simulations described in Sweeting et al. (2011) and the battery models derived in the following sections. A flow diagram for the model is given in Figure 5.5 and the operation is outlined below. Further background data on some of the equations used can be found in Larminie and Lowry (2003).



Figure 5.5 Flow diagram for BEV use phase model

The model begins by calculating the power and velocity necessitated at the vehicle"s wheels based on the inputted vehicle parameters and driving cycle. This is then converted into power and rotational speed requirements from the motor, allowing for the drivetrain ratio and efficiency. These parameters are then used to calculate the motor efficiency and required input power. This power requirement, together with that for any auxiliary draws, is fed to the battery model. Based on equations for the voltage and resistance, for each of the battery packs assessed, the effective energy removed from the battery is calculated. These operations are repeated until the battery capacity, calculated from the specific energy and inputted battery mass contained in the vehicle, is depleted to set limits. The battery model is then used to find the battery efficiency and input energy needed to restore the removed charge. This input is then converted into an energy requirement from the grid by incorporating charger losses.

Data from the motor and battery models was checked to ensure it was within the capabilities of the simulated components.

The following sections present the vehicle parameters used in the simulations and provide more information on the battery/charger models. Trial data is then used to validate the use phase model and provide approximations for possible real-world driving requirements. Finally the data used for the comparison conventional vehicle's use phase is presented.

5.8.1. Vehicle parameters

Table 5.5 gives the parameters which were used to simulate the baseline BEV over the NEDC.

Parameter	Value
Vehicle mass excluding traction batteries and 100kg load (see below)	1214 kg
Coefficient of drag	0.29
Coefficient of rolling resistance (for energy efficient tyres)	0.007
Vehicle frontal area	2.3m ²
Average power draw by accessories	250W
Road incline	0°
Percentage of braking energy recouped	50%
Drivetrain efficiency (excluding battery, motor and electronics)	95%
Density of air	1.25kg/m ³
Gear reduction ratio	8

Table 5.5 Values used to simulate BEV use phase

The total vehicle mass used for the in-use calculations was based on the powertrain and glider vehicle values, given in Sections 5.4 and 5.5 respectively, to which the battery mass was added. For consistency with consumption figures quoted by manufacturers an additional 100kg was applied in line with Commission Regulation No 101. The battery mass was left as a variable that was adjusted for each of the batteries assessed to enable the vehicle range, 175km, set in the functional unit (see Section 5.3.1).

The coefficient of drag, vehicle frontal area, gear ratio and motor/inverter efficiency map were based on values for the Nissan Leaf to help comparisons with test data, see Section 5.8.5 (Nissan, 2010; Sato, et al. 2011). The accessory power draw was also based on the Nissan Leaf, using the author's measurements from the on-board energy information display, with all unessential auxiliaries turned off in accordance with Commission Regulation No 101. Details on the other parameters are given in Sweeting, et al. (2011).

The model was adapted so that it calculated the battery energy efficiency (see Section 5.8.3) and permitted selection between simulations for each of the three lithium-ion variants assessed (see Section 4.3.1).

5.8.2. Vehicle charging

Chargers in the UK typically range from 2.4kW (10A), for those using standard supply sockets (with approximately 3.2kW (16A) and 7kW (32A) rates being common upgrades), to around 50kW for specialise fast charging units (British Gas, 2013). The maximum available rate however may not always be used, with that supplied by fast chargers reducing substantially as the battery state of charge (SOC) increases.

In this assessment a baseline charging rate of a constant 3.2kW was used to represent that of current standard dedicated home chargers (Charging Solutions Ltd, 2013).

Typical energy efficiencies, totalling around 83% (90% and 92% for chargers and batteries respectively), have been used to model the losses associated with electric vehicle battery/charger systems (Campanari, et al. 2009; Gerssen-Gondelach and Faaij, 2012; Pollet, et al. 2012). This represents a substantial loss, which significantly abates the high efficiency offered by BEV motors. To check this assumption, data supplied by Nissan for their Leaf model (see Table 5.6) was employed (Nissan, 2010). If the entire battery capacity of 24kWh was used to meet the quoted range of 175km, a maximum average energy of 137Wh/km would be available. This suggests an efficiency of 79%, which is similar to that found for other BEVs (Cenex, 2010; Bütler and Winkler, 2013), when compared with the manufacturer value for energy taken from the socket (173Wh/km). This indicates that the charger/battery system efficiencies of current BEVs could be even less than 83%.

Parameter	Value
Battery capacity	24kWh
Manufacturer electricity consumption from socket over NEDC	173Wh/km
using on-board charger i.e. including charger/battery losses	
Range over NEDC	175km

Table 5.6 Data for 2010 Nissan Leaf

The above approximations do not indicate where in the system the inefficiency arises and for example, battery efficiency will change with power draw and thus driving cycle. Comparisons of trial data (see Section 5.8.5), for the average energy consumption using the on-board charging system against that found using the outputs of off-board units (which were assumed to not include charger losses), suggested the majority of the inefficiency may result from the charger. However, further data is needed to provide a more accurate

picture of the losses and to establish how far this seemingly large area of inefficiency can be reduced.

For this assessment a default static charging/battery system efficiency of 85% was assumed. This was intended to encompass all the losses, between the grid connection and final battery output, except those resulting from the battery resistance. These were addressed separately in the battery model (see Section 5.8.3) and allowed for some of the effects of variations in power demand, SOC and cell type on the battery efficiency. Therefore the total modelled charging system efficiency, including that of the battery, was below 85%, the precise extent of which depended on the above factors.

5.8.3. Battery model

This section describes the formulation of the models used to simulate the batteries and estimate their energy efficiency over varying conditions.

Battery model construction

The voltage of a battery varies with the SOC and load, which in turn affects the current for a given power demand. Therefore, to calculate the current and efficiency, data on the battery voltage is required. This was calculated by fitting polynomials to the voltage discharge profiles of suitable lithium-ion cells, in order to define an expression for the open circuit voltage in terms of the cell"s SOC, as described for other battery types in Larminie and Lowry (2003). To approximate how the voltage was affected by current draw, the battery was modelled as a simple voltage source and resistance, see equation (5.1), and values for the cell internal resistance were derived based on published discharge profiles for differing current draws.

$$Voltage = V_o - R_{cell}I \tag{5.1}$$

Where:

I is the current draw (A).

R_{cell} is the cell internal resistance (Ohms).

V_o is the open circuit voltage (V).

The LMO cell model was based on data for those fitted to the Nissan Leaf (Ikezoe, et al. 2012). Figure 5.6 shows the simulated voltages superimposed on this data. The capacity of these cells was shown to only reduce marginally as the current increased. In the model the discharge capacity was therefore taken to remain constant, i.e. no Peukert effect has been accounted for. However the simulated usable energy supplied does reduce as the power draw increases due to the batteries internal resistance.



Figure 5.6 Simulated and manufacturer voltage profiles for LMO cell

Figure 5.6 shows the simulated data provides a reasonable fit, with the exception of the values for high current draws at low SOC, i.e. nearing full discharge capacity. The simulations used a fixed value for the internal resistance of 2.4mOhm, which is similar to the 2mOhm given in the manufacturer's specification for the cells. However, cell resistance tends to increase at low SOC, which could explain the inaccuracies found in this region (Nelson, et al. 2002; Rong and Pedram, 2006; Culcu, et al. 2009; Anseán, et al. 2013).

Modifying the model by incorporating a polynomial to provide an estimation of how the resistance alters with SOC resulted in the voltage profiles shown in Figure 5.7. The resistance profile derived to attain these results is shown in Figure 5.8 and the polynomial used is given in equation (5.2), where DOD is the depth of discharge (i.e. 1-SOC).





Figure 5.7 Simulated voltage profiles for LMO cell with variable resistance



Figure 5.8 Values used in LMO cell model

This modification to the resistance significantly improved the accuracy at low SOC, see Figure 5.7 compared to Figure 5.6, giving good estimates of the voltage, particularly over the 80% charge range used in the simulations (see Section 2.3.1 and Figure 5.8). For example the discrepancy, seen for the 90A discharge at 28Ah discharge capacity (\approx 15% SoC) Figure 5.6, over halved from approximately 0.07V to 0.03V compared to the

published curve. However, there were several limitations and assumptions associated with the model:

- The transition period in the voltage as the current alters was not accounted for.
- The resistance profile and capacity were assumed to be unaffected by the discharge rate.
- The resistance was assumed to be the same in charge and discharge.
- Temperature effects on the results were not incorporated.
- The data used to construct the models, for each of the lithium-ion chemistries, was taken from large cells of the types used in vehicle applications. However, other values may be obtained if, for example, data from different manufacturers or cell sizes were used.

Equations for the voltage and resistance of the nickel cobalt manganese (NCM) and lithium iron phosphate (LFP) cells were generated in the same manner using test data presented in Mulder, et al. (2013) for large cells. The discharge capacity for NCM cells appeared to have greater variation with the discharge rate, which resulted in the model being less accurate than that shown for the LMO cell in Figure 5.7. Within the SOC window and anticipated current range utilised in the model, the voltage profiles generated were still reasonable. However the higher capacities shown for low current discharges were not accounted for.

The internal resistance of lithium-ion cells tends to increase as the cells age, which will affect their efficiency (Rong and Pedram, 2006; Nelson, et al. 2011b; Ecker, et al. 2012). Therefore, to provide a simplistic approximation of some of the effects of aging and allow the impacts on the cell efficiency to be assessed, a variable multiple for the internal resistance was incorporated into the model. Due to the limited SOC range used in the model, the useable energy was assumed to remain constant with aging.

To convert the cell resistance to that of the pack, equation (5.3) was used which is based on the cells resistance being approximately inversely proportional to the capacity (Larminie and Lowry, 2003; Mulder, et al. 2013).

$$Pack resistance (Ohm) = (N_{cells} * C_{cell} * R_{cell}) / C_{pack}$$
(5.3)

Where:

N_{cells} is the number of cells in series needed to meet the specified pack voltage.

 C_{pack} is the pack capacity calculated for the vehicle to attain the range set in the functional unit (Ah).

R_{cell} is the cell resistance calculated as described above (Ohms).

 C_{cell} is the capacity of the cell to which the resistance (R_{cell}) relates (Ah).

In the model a nominal pack voltage of 360V was used, which is similar to that employed in current BEVs (Matthe, et al. 2011; Ikezoe, et al. 2012). Based on the necessitated vehicle battery pack energy, this enabled the number of cells and capacity to be calculated for each of the chemistries, assuming the capacity could be varied to suit. Vehicle battery packs may also contain cells connected in parallel to increase the capacity. Differences between the resistances of parallel cells and their connectors can affect the performance of a battery pack, for example decreasing the lifetime (Gogoana, et al. 2014). In the model all the cells were assumed to be equal and the total resistance was calculated based on the pack capacity, equation (5.3). Therefore the model only considers a single series string, because the assumption of parallel cells to reach the required pack capacity will not affect the equations used.

Battery system efficiency

Battery energy efficiency was introduced in Section 2.3.2 and identified as a potentially significant parameter both between different batteries and on the whole life energy requirements of a BEV. Efficiency can vary due to a variety of reasons, for example changes in the temperature and battery age (see Section 2.3.2). However equation (5.4) provides a simple relationship showing how the efficiency is affected by increased current draws and resistances, where P is the power demanded from the battery (Burke and Miller, 2011).

Energy efficiency =
$$P / (P + I^2 R) = P / (V_o I)$$
 (5.4)

Figure 5.9 shows the efficiency (cells only) predicted by equation (5.4) for several constant power discharge rates, using data for LMO cells and a pack capacity of 24kWh. The results were generated by running iterations a one second intervals until a minimum SoC was reached, based on the ratio of charge removed to the total pack capacity. Data for the input parameters was generated using the expressions derived for the battery voltage, discussed above, together with equations (5.1) and (5.3) to find the pack current and resistance respectively.



Figure 5.9 Simulated LMO cell efficiency for pack under constant power discharges

The results indicated the efficiency dropped by around 10% as the power draw increased towards 120kW (approximate peak draw for a reasonably powerful "C" segment vehicle and auxiliaries). However, high powers are only likely to be required for short periods, i.e. under maximum acceleration at speed. The efficiency drop at low states of charge also indicates the potential gains of limiting the usable SOC window as shown in Figure 5.8.

Re-running the model including an additional resistance of 0.05 Ohms to approximate that of the other components, for example the connections and cabling between the cells and battery (Larminie and Lowry, 2003; Miyazaki, et al. 2008), gave the results shown in Figure 5.10. Note the simulations were stopped at 15% SOC due to rapid decreases in the efficiencies. This figure also incorporates results for the charge phase, using an additional static charging/battery system efficiency of 85%, see Section 5.8.2.



Figure 5.10 Simulated LMO battery pack and charger system efficiencies

For the baseline charging rate of 3.2kW and 0.95 to 0.15 SOC window (Figure 5.10), these simulations gave an average combined charge/discharge cycle system efficiency (i.e. including the charger, battery and connections/cabling), of approximately 84% for a constant 5kW discharge, dropping to 70% for a 120kW discharge rate. Results using the data for NCM and LFP cells indicated little change in the efficiencies at low powers, but slight improvements at high draws.

To approximate the effect of aging, the cells internal resistance was doubled based on results from Ecker, et al. (2012). For the LMO pack at a constant power draw of 20kW this caused the combined system efficiency to drop by approximately 2%.

The effect of employing a 50kW fast charger was shown to be a combined system efficiency drop of around 4% (assuming the rate was held constant throughout the charge and not including any cooling requirements).

The results given above are only to provide an indication of the model outputs and they will vary depending upon, for example, the data used to construct the model, the charge/discharge rate and the model accuracy. The values from actual cells may therefore differ. Further discussion on the model results is given in Section 7.2.

5.8.4. Model validation

To check the accuracy of the use phase model, it was run over the NEDC with a proxy for the battery mass to give a vehicle mass equal to that of the Nissan Leaf, approximately 1525kg (1625kg with additional 100kg for consistency with test regulations). The energy consumption from the battery, for this simulation, matched the 137Wh/km derived from the manufacturer data in Section 5.8.2 to within 1%. Larger differences in the value for the total energy supplied (i.e. from socket) were found due to the slightly higher charging/battery system efficiency used. However, reducing the default charging/battery efficiency in line with the large losses found for the Leaf (see Section 5.8.2), resulted in values that matched the manufacturer data of 173Wh/km with a similar accuracy.

5.8.5. Driving cycles

The NEDC tends to underestimate the energy consumption of vehicles compared to that found during typical actual vehicle usage, as discussed in Section 3.3.1. This could result in the findings of whole life assessments being more biased towards other phases of the

lifecycle than may actually be the case during real-world usage, due to underestimations of the in-use phase.

To study the potential significance of the driving cycle, results for a scenario where the use phase energy consumptions were adjusted to approximate those from real-world test data were included. The test data was based on trials involving a Nissan Leaf using a Brennenstuhl PM 230 energy monitor, connected between a standard 13A socket and the vehicle's on-board charger, to record the energy supplied. To help provide a sample of potential real-world use scenarios the trials encompassed a variety of different drivers and trips. They were conducted in and around Oxford between November 2012 and January 2013, with auxiliary systems e.g. heating, demisting, and wipers, employed as necessary. The trips encompassed a range of speeds, roads and traffic conditions, ranging from high speed duel carriageway sections, through free flowing single carriageways with typical speeds of 48 to 97kph, to low speed congested areas with frequent stops.

The energy demands will depend upon the location, weather, vehicle and driver due to factors such as different acceleration rates, speeds and use of auxiliary systems. The timing of the trials for example fell over months which are typically colder than average for the location. This is likely to have led to greater use of heating and demisting systems than for the yearly average. Therefore, as with the results attained using the NEDC, the data from these trials only provided values for a fragment of the many possible scenarios.

The average energy consumptions measured, along with those for some specific tests, are given in Table 5.7. These show that the manufacturer's test figure of 173Wh/km, attained for the NEDC, can be obtained with careful driving and limited usage of auxiliaries. On average though the consumption was 35% higher, with values approaching 60% greater attained for journeys involving substantial use of the auxiliary systems (e.g. frosty mornings). The use of auxiliaries is particularly problematic because they can result in large power draws which are independent of the vehicle's speed, as discussed in Sweeting, et al. (2011). In extreme circumstances, such as in stationary traffic with heating/demisting systems on, this may result in the auxiliaries consuming the majority of the energy, and very high per km consumptions.

To give some perspective to the figures in Table 5.7, values recorded for a desktop computer system showed a consumption of over 2kWh/day whilst on and still over 0.5kWh/day when shut down. These are effectively equivalent to travelling 8.5km and 2km respectively, for the average trial data, or 11.5km and 3km over the NEDC.

Factor	Value
Energy consumption from wall socket, averaged over trials covering	234 Wh/km
1607km	
Energy consumption for trials with all auxiliaries off and limited	169 Wh/km
accelerations to provide approximation of NEDC conditions	
Energy consumption for trials with extensive use of demister/heaters	273Wh/km
Maximum demister power consumption from on-board readout	4.5kW
Energy consumption using off-board Chargemaster fast charging unit.	189Wh/km
Estimated from energy supplied according to inbuilt charger readout.	
Note accuracy unknown and expected to exclude charger losses.	

Table 5.7 Data from trials using a Nissan Leaf

The 35% energy increase over the NEDC test data fell within the range found for conventional vehicles, but was significantly above the average of 23% reported by Transport and Environment, (2013). Given that the test data is obtained with the auxiliaries switched off and the potential effect these can have on BEV energy consumption, as discussed above, suggests this higher than average increase may be anticipated.

Therefore to approximate the potential effects of real-world conditions, the values attained over the NEDC were increased by 35%. To allow rough calculations of how this may influence the results from the battery model, the European Urban Driving Cycle was used. The velocity profile of this cycle was subsequently adjusted by a multiple, as described in Sweeting, et al. (2011), to give the required 35% energy consumption increase from the grid. The calculated multiple using the LMO pack was 1.85, which was employed for all the battery chemistries. This gave a maximum speed of 93kph (57mph) and 0 to 96.6kph (0-60mph) acceleration time of 27 seconds (based on extrapolation of the longest acceleration period). These performances are well within the capabilities of many electric vehicles, e.g. the Nissan Leaf.

5.8.6. Conventional vehicle use phase

To provide approximate data for a similar conventional vehicle, manufacturer figures for the fuel consumption of an efficient diesel 2013 Peugeot 308 HDI 92 hatchback over the NEDC were used, 4.0 litres/100km. This vehicle was selected because it has a similar size and the same frontal area/drag coefficient product as that used for the BEV.

6. BATTERY MODEL RESULTS AND DISCUSSION

6.1. Introduction

This chapter contains a selection of the results, generated from the battery model described in Chapter 4, along with a discussion of the findings. The results are centred on the functional unit for the battery model, which was the production and end-of-life (EoL) treatment of one kg of lithium-ion battery pack (see Section 4.3.1). The segregation of the battery, from the whole vehicle model, allowed comparisons with existing battery life cycle assessments (LCA).

Together with Chapter 4, which detailed the development of the model, this Chapter addressed the first three objectives of the project (Section 1.4.5). These were the discrepancies in existing assessments, the effects of variables and the impacts of recycling. This chapter has thus been divided into sections which address each of these. Prior to these, the limitations of the methodology are discussed and a brief section on the interpretation of the results is provided. These should help ensure the limitations of the findings are appreciated and minimise the chances of any misinterpretation. The final sections of the chapter provide a brief analysis of the possible effects of alternative impact categories and summarise the findings.

Chapter 7 then builds on this by analysing the battery in the context of its intended use, i.e. in a BEV.

6.2. Limitations

This section summarises the main limitations of the methodology employed. More specific details on the limitations of individual inputs and assumptions, used during the development of the models, are given in Chapters 4 and 5. The effects these have on the results are discussed in the relevant sections that follow.

The life cycle model constructed aimed to be as representative as possible of the actual material flows and processes incurred during the life of a BEV. However, the base model only represents a snapshot of the numerous possible variables found amongst vehicles, their usage and their production/recycling. Some of the key variables were parameterised, particularly for the battery where the research was focused, to enable their effects to be studied. This still left many possible areas where discrepancies could arise between the results predicted by the model and those achieved in the real-world. These areas included:

- Discrepancies in the battery production processes. These resulted from limited data on lithium-ion battery production details, the development rate of the technology and the different processing routes possible for many materials/components.
- Differences in the production impacts of the materials. The base input materials were modelled primarily using datasets from GaBi, which often represent average values for geographical regions. Throughout the assessment average values for Europe, where appropriate and available, were employed. It should therefore be appreciated that the impacts could vary depending upon the particular facility, or location, the materials are sourced from. The impacts will also vary with the accuracy of the dataset (e.g. due to measurement errors and the assumptions used) and time (due to the introduction of new processing technologies for example). This introduces potential temporal variation into the input data. Further details on some of the general limitations in LCAs are identified in Baitz, et al. (2011).
- Alterations in the vehicle's usage profile, e.g. different driving cycles and vehicle loads.
- Variations in the glider vehicles, e.g. different materials, trim levels and sizes.
- Differences in the charging system efficiency.

The primary metric quantified in the results was global warming potential, presented in kg of CO₂ equivalents, see Section 4.3.3. However evaluations involving alternative impact categories, such as human toxicity or resource depletion, will affect the results and could alter the optimal choice in comparisons of powertrains. Limited inventory data for many of these categories, coupled with the use of differing characterisation methods (Finnveden, et al. 2009), was expected to result in their values often being far more uncertain than those for global warming potential. It was possible to generate values for some of these metrics using the constructed GaBi model and results for several alternative impact categories are given in Section 6.7. However further work is needed to better quantify their impacts.

The purpose of this research project was not to provide definitive values or final conclusions upon what powertrain is the optimal choice. However, it was intended to improve knowledge and understanding of the areas given in Section 1.4.5. This should enable more holistic assessments to be developed, which permit increasingly robust conclusions, by helping identify what situations and parameters, or ranges of these, need to be defined and their potential effects on assessment findings.

The research was focused on the direct impacts and variables associated with the production, use and disposal of BEVs in the near term. However, there are several additional factors that should be appreciated when comparing powertrains. These include:

- The repercussions on material supply and production impacts caused by the large scale use of alternative technologies, such as the effects on rare earth metals demand caused by utilising permanent magnet motors (see Section 1.2.3).
- The external economic and social costs arising from damage to human health, materials and crops due to vehicle emissions. For example the use of alternative vehicles, such as BEVs, could eradicate tailpipe emissions in urban areas, thereby improving wellbeing and reducing health care costs.
- The impacts associated with the provision and construction of the infrastructure needed for alternative fuels, such as electricity and hydrogen (see Section 2.1).

Further details on some of these factors are given in a paper by the author, Sweeting and Hutchinson (2013) see Appendix A, which investigated aspects that can affect the findings of vehicle assessments.

These additional considerations have not been included in the analyses due to time constraints and the difficulties in quantifying factors such as external costs (Defra, 2011). However future work could expand the model to encompass them.

6.2.1. Results interpretation

A degree of uncertainty will exist in complex LCAs, for example resulting from the use of assumptions/estimations and the incorporation of background data, whose precise derivations may be unknown (Lloyd and Ries, 2007; Finnveden, et al. 2009; Baitz, et al. 2011).

Due to these considerations and the limitations discussed above, it should be appreciated that there is a degree of uncertainty in the results presented here. The results should therefore be viewed as a guide whilst considering the particular set of scenarios they aim to evaluate. To quantify some of this uncertainty, sensitivity analysis was performed on several factors found to potentially vary significantly. The findings of which are discussed in the sections below.

Considering the uncertainty for some factors in the overall model, the differences resulting from several of the analysed parameters may appear small. However, in comparisons

between parameters the uncertainty should remain equal for all the unaltered values, i.e. any resulting under or overestimations from these should be equal. This means the relative difference between the results, shown for variations in a particular parameter, should still provide a reasonable indication of the anticipated effects.

Only a selection of the results for the most noteworthy variables have been presented here, due to the number of possibilities and combinations of them. However alterations to any of the materials or processes will affect the findings to some degree. For some variables the results for approximate best and worst case scenarios have been given. This approach was taken to indicate the potential range, but in most cases the actual values are anticipated to fall somewhere between these two extremes.

In this chapter, and those that follow, impacts are taken to refer to those of carbon dioxide equivalent emissions (CO_{2e}) , unless otherwise stated.

6.3. Baseline results

This section presents the results for the baseline scenario, together with a discussion of the main contributors. The baseline values are conferred in Chapter 4 but, for clarity, those used for the main variables are listed in Table 6.1. These values have been utilised for all the results unless otherwise stated.

Factor/variable	Baseline value
Recycling fraction/credits (battery model only)	0 (i.e. no recycling/EoL treatment)
Cell mass percentage of total pack	60%
Anode active material production	Artificial graphite using EU grid mix
	electricity
Transportation distance for products in Europe	500km

Table 6.1 Baseline values used in model

Figures 6.1 and 6.2 present the results for the production of one kg of battery pack using the baseline values and each of the cell chemistries, i.e. lithium manganese oxide (LMO), lithium nickel cobalt manganese (NCM) and lithium iron phosphate (LFP). The final assembly/transportation value refers only to the battery pack assembly, as defined in Section 4.4.11 and transportation of components to the final battery manufacturing facility.



Figure 6.1 Results of baseline scenarios for each of the battery chemistries



Figure 6.2 Percentage split in CO_{2e} emissions for baseline scenarios

The results show the cells represent the majority of the CO_{2e} emissions, 63-68%. This is slightly above their mass percentage of 60%, indicating that they have above average impacts compared to the whole of the battery pack. A further breakdown of the cells, Figure 6.3, shows that the majority of the impacts result from the cathode and anode assemblies, around 50% and 30% respectively for all the cell types.



Figure 6.3 Breakdown of cell impacts for baseline results

The next major contributor to the total pack is the battery management system (BMS), of which 86% results from the circuit boards, further details of which are given later. The other main contributors are the battery and module casings. In the case of the battery housing, the impacts result from the large mass of this component, 25% of the pack, which is approximately 2.5 times higher than its corresponding relative impacts. The large quantity of steel in this component lends itself to recycling which will reduce the impacts. The module casing effects result chiefly from the aluminium used which has relatively high production influences, see following section.

The results in Figure 6.1 indicated only reasonably modest differences, on a per kg manufactured basis, between the three different lithium-ion battery chemistries evaluated. The NCM pack is shown to exhibit the highest impacts, approximately 16% above the LFP pack with the lowest.

The trend between the cell impacts matched that of their specific energies, see Table 4.1. This indicated that, from the cells analysed here, there is a general correlation between increasing production impacts and higher specific energies. The rate of change of these concomitant effects was found to differ, with energy increasing faster than production impacts. The extent of this effect resulted in a reversal of the findings between the different packs, when viewed on a per energy basis as shown in Figure 6.4. Here the impacts of the NCM pack are now approximately 20% lower than those of the LFP, which has implications for the selection of vehicle batteries as discussed in Chapter 7.



Figure 6.4 Comparison of results on a per mass and per energy storage basis

This suggests that it is likely to be beneficial, in terms of CO_{2e} emissions, to opt for increased specific energies where a given storage capacity is required. However, analysis of more cell variants is required to verify this trend, it does not account for other factors (e.g. lifetime) and caution should be observed because, some changes to increase energy may have dramatic effects on the production impacts. For example the use of a chemistry which although may offer energy benefits, necessitates stringent cooling requirements or additional BMS controllers to ensure safe operation, which incur large additional impacts.

6.3.1. Main contributors to the impacts

To identify the main individual contributors, weak point analysis was performed using the GaBi model to probe into the constituent inputs. The weak point threshold was set to identify any processes/materials which contributed more than 5% of the overall CO_{2e} emissions. The factors identified by this, for the LMO battery pack, are given in Table 6.2 and further discussion of each is provided in the following subsections. The BMS and anode graphite are not covered here, but are included in the discussion of variables in Section 6.4.

Material/process	Percentage of total impacts
Cathode active material (LiMn ₂ O ₄)	20.9%
BMS - circuit boards only	10.7% (of which 5.3% results from the production of the bare printed wiring board)
Anode graphite	9.2%
Electricity used in cathode production	7.7%
Aluminium used for module cases	7.2%

Table 6.2 Main contributors to battery pack impacts

Cathode active material

There is a large degree of variability surrounding the production of the cathode active materials for lithium-ion batteries, due to the variety of materials and deficit of primary data, as discussed in Section 4.4.4. Considering the importance of the cathode active material, these variables could have a significant bearing on the findings. For example, the results of this assessment found approximately 6kg and 11kg of CO_{2e} emissions per kg of the LFP and NCM cathode active materials respectively. These results only represent approximations for one particular set of synthesis routes and there are many proposed routes and various precursors for each of the active materials which could yield different results (Jugović and Uskoković, 2009; Jung, et al. 2012; Pan, et al. 2013).

All the cathode active materials represented a large proportion of the total impacts. However their proportions and main contributors varied, as shown in Table 6.3.

Cathode	Cathode active material	Main contributors to active material
material	percentage of total pack CO _{2e}	impacts
LMO	21%	Production of Mn ₂ O ₃ precursor 59%
NCM	26%	Production electricity 31%, nickel 39%
LFP	15%	Electricity used in production 44%

Table 6.3 Main contributors to the cathode active material impacts

The appearance of the production electricity as a major contributor for the NCM and LFP materials, suggests that the benefits of recycling may be limited, unless materials can be reclaimed in a form above that of the base precursors (i.e. as an intermediate or final substance which requires less processing energy to attain the final active material). The high contribution of the Mn_2O_3 precursor to the LMO cathode warrants further analysis, to

ensure the impacts are representative, and study the effects of different synthesis routes. For example those outlined in Manev, et al. (2003), which uses alternative precursors for Mn_2O_3 and Iwata, et al. (2013), who note the possible use of different manganese compounds altogether for producing $LiMn_2O_4$. Unfortunately a lack of data on the production impacts of these routes and the time constraints of the project precluded their quantification here.

The supply of lithium, in the form of carbonate, was found to be a notable factor in all the cathode active materials, representing 7 to 8% of their impacts. However it was not one of the main contributors as shown in Table 6.3. Further discussions of lithium's impacts are provided in Section 6.6.2.

Cathode production energy

The electricity used in the production of the coated cathode assembly is a substantial contributor. Most of the electricity inputs resulted from approximations based on machine specifications for coating and drying of the active material. This is thus an important area to obtain primary battery manufacturing data for to verify the results. The choice and amount of solvent could also have a large influence on this figure, see Section 4.4.3. For example, if the solvent ratio used could be substantially reduced in mass production, it should be possible to mitigate the drying energy.

Module casings

The aluminium module casing represented 7.2% of the impacts and 5% of the mass. Redesign of the battery pack could help reduce this figure, either through the use of less or different materials. This aluminium is a good candidate for recycling, which could reduce the impacts to less than 3%, assuming 100% recovery and neglecting dismantling requirements.

6.4. Effects of variables

This section presents the results of the sensitivity analysis on the main variables identified. Further analysis of the variables that are more relevant to the in-use phase of the battery, i.e. lifetime and efficiency, are addressed in the following chapter on the whole vehicle model. Unless otherwise stated all the results are based on the pack containing LMO cells and baseline parameters.

6.4.1. Transportation

The transportation impacts, as defined in Section 4.3.5, were found to represent 1.6% of the total CO_{2e} emissions. This value only represents the additional transportation of the input materials, given in the inventory in Chapter 4, to hypothetical European manufacturing facilities and does not include any values contained within the input datasets, e.g. for transport of their precursors.

To assess the influence of the default European transportation, the model was re-run with the average distance doubled to give 1000km. This large value (for comparison the standard transportation suggested by Ecoinvent for various materials consumed within Europe only ranges up to 700km (Frischknecht, et al. 2007)) resulted in the transportation still representing less than 3% of the total impacts.

This suggests that, even if the actual transportation values deviate substantially from the baseline, they are only likely to have a relatively small effect on the overall results.

6.4.2. Cell mass fraction

The potential discrepancies in models, regarding the mass fraction the cells were assumed to represent of the total pack, were discussed in Sections 3.4.1 and 4.4.1. Figure 6.5 shows the results for scenarios where the cells are reduced to 50% of the pack mass and increased to the 80% used in many existing assessments.

On a mass basis this gave a reduction in impacts of around 2%, when the cells were reduced to 50%, and an increase of 4% when they were increased to 80%, relative to the default mass percentage of 60%. However, altering the cell fraction will also affect the overall pack specific energy. This influence resulted in the higher production impacts associated with increased cell fractions being more than offset on an energy storage basis, assuming the cell specific energy remains constant, see the per kWh values in Figure 6.5.

These findings suggest that the assumption regarding the cell mass fraction has a relatively small effect on the CO_{2e} emissions per kg of battery pack produced, considering the alterations it makes to the pack. The assumption should therefore not have a large effect when comparing the results with other battery LCAs on a per mass basis. However, on an energy basis the influences are far more significant, with a reduction of approximately 22% found when the cell mass fraction increase to 80%, compared to the baseline.



Figure 6.5 Influences of modelled cell mass fraction

The cell mass fraction and specific energy are therefore important factors that need to be considered to ensure consistency, when capacity is involved in comparisons between assessments. For example, at the vehicle level where a specific battery pack energy is required.

Due to the linear relationship used in the model, all the non-cell pack components are reduced as the cell mass increases. This meant that the packs with higher cell contents effectively contained a reduced BMS mass. Considering the importance of the BMS on the total findings, this may have resulted in underestimations of the impacts for the packs with high cell fractions. Running the model with the BMS mass held constant, showed this did have a noticeable effect, increasing the effects on a per kg and reducing them on an energy basis. Despite this, the differences still remained substantial on an energy basis, with an 18% reduction found when assuming an 80% cell fraction.

6.4.3. Anode active material

Graphite was assumed as the anode active material for all the scenarios. However it can be produced by two completely different routes, natural and artificial, see Section 4.4.3. The artificial route is very energy intensive, which results in the impacts being highly sensitive to the energy source. Considering it is one of the largest single contributors to the overall impacts at over 9% (see Table 6.2), the production route could have a notable bearing on the results.

The effects of the production routes are shown in Figure 6.6. This indicates over a 6% reduction, in the total impacts, if natural graphite is used in place of artificial produced using EU grid electricity. The benefits shown for using hydroelectricity, for the graphitisation process, also suggest significant detrimental effects would be experienced if artificial graphite was produced using electricity with higher emissions than the EU grid mix.



Figure 6.6 Effects of graphite production assumptions

6.4.4. Battery management system

The BMS was identified as a main contributor, as found in previous studies (see Section 3.4.1), due to the impact of the circuit boards. This was despite the revisions to the inventory, discussed in Section 4.4.10, which lowered the circuit board impacts, and the fact that it represented only 0.7% of the pack mass.

Around half the circuit board impacts were found to be attributed to the manufacture of the bare board (Ecoinvent process "printed wiring board, surface mount"). This meant the components and their fitment only represented half the impacts. Investigation into the impacts of bare circuit boards, to ensure the representativeness of the process and identify any areas where mitigation is possible, is therefore a valuable area for further work. To provide an indication of the influence of the board, the Ecoinvent process "printed wiring board, through-hole", was employed as it exhibited far lower impacts. This substituted the data for a "surface mount board", which was selected as the default to match that found in the BMS of a LiFeBATT battery pack (Section 4.4.1).

The results of this alteration, along with those for variations in the baseline circuit board mass by $\pm 50\%$, are given in Figure 6.7. Overall the change in the modelled bare wiring board process reduced the impacts by 3%, highlighting the importance of the assumption surrounding the BMS background data.



Figure 6.7 Effects of changes to the BMS circuit board

Considering the 0.8% BMS circuit board mass, of the total pack, measured from the LiFeBATT pack (see Section 4.4.1) and 0.6% to 0.7% reported in Buchert, et al. (2011), the 0.7% used in this assessment was judged to be a reasonable approximation for current vehicle battery packs. However the requirements can vary for a variety of reasons, e.g. due to changes in the number of cells, pack size and chemistry (Element Energy, 2012). The mass alterations shown in Figure 6.7, which reduced the BMS circuit board fraction down to a value similar to that estimated in the LCAs by Notter, et al. (2010) and Majeau-Bettez, et al. (2011), resulted in approximately \pm 5% changes in the total impacts. This showed that the assumed circuit board mass could have a significant influence on assessment findings.

6.5. Recycling

Figure 6.8 shows the effects of including recycling on the battery pack. The results presented are for the maximum recycling scenario, i.e. assuming all batteries are collected and a steady state where the materials from recycling one battery pack are all available to substitute those used in the production of an identical pack, effectively a closed loop scenario. However, increasing production and changes in battery constituents will result in a lag between demand for production materials and those available from battery EoL recycling, see Section 4.3.5.



Figure 6.8 Effects of end-of-life phase on the battery pack impacts

Due to the relatively high processing requirements of the modelled hydrometallurgical process and limited amount of valuable metals, particularly in the LMO and LFP cells, the reductions are limited. However, due to the credits from reclaimed cobalt and nickel in the NCM pack, this showed an 11% reduction. This resulted in narrowing the gap between the chemistries, depicted in Figure 6.1, to a maximum of 7% between the NCM and LFP packs.

The LFP pack showed marginally greater benefits than the LMO, which resulted from the larger amounts of aluminium and copper in the cells and the adverse impacts of manganese recovery, see below.

Interrogation of the results revealed that the bulk of the recycling benefits were attributed to the materials reclaimed from the non-cell components, predominantly the pack casing, aluminium module housings and copper. In the case of the LMO and LFP cells themselves they were found to have negative benefits, due to the credits for the reclaimed materials being insufficient to compensate for the recycling requirements. This effectively meant they reduced the benefits attained by the non-cell components. However, this situation could be altered considering the following:

- The processing requirements were based on trials and may be reduced by future refinements and economies of scale.
- The modelled hydrometallurgical recycling route was selected due to the potential for high recovery rates. Different processes may have lower requirements and give

increased overall emission reductions. However this may be at the expense of the recycling rate.

• The form and method in which the materials are recovered can differ. For example are the materials produced from recycling the same as those used during battery production or are lower grades obtained, which cannot be directly reused but may be easier to recover.

Two major considerations, identified in the modelled hydrometallurgical recycling route for the LMO battery pack, were the treatment of the anode graphite and manganese from the cathode. This was due to their modelled EoL processing having net detrimental effects, specifically incineration with electricity generation for graphite and manganese recovery in carbonate form, see Section 4.5.4. Re-running the simulations with the assumption that both these materials were instead sent to landfill, resulted in the benefits of recycling increasing from 2% to over 6% for the LMO pack, see Figure 6.9.



Percentage reduction in CO_{2e} emmissions over no EoL treatment

Figure 6.9 Effects of end-of-life assumptions on LMO battery pack impacts

The above considerations suggest that the benefits of recycling can be increased. However, unless significant changes to the processing are introduced, e.g. to enable the direct recovery and reuse of cathode active materials or to substantially reduce the processing requirements, recycling is only likely to offset a limited fraction of the production CO_{2e} emissions.

This same trend was found for primary energy demand, but potentially greater recycling gains were shown for other impact categories, see Section 6.7.

6.6. Comparison with existing battery life cycle assessments

This section compares and contrasts the findings of this assessment with those in the existing literature; to identify some of the reasons for the large variations reported. Firstly the baseline overall findings are compared and then specific factors of interest are addressed.

6.6.1. Overall findings

Differences in the assumed battery specific energy used amongst assessments which model similar chemistries can introduce substantial variations in the findings. To allow for this, comparisons on both a per mass and a per energy basis are presented where possible, Figure 6.10 and Figure 6.11 respectively. The figures revealed that the trends amongst the different assessments were similar for both bases. Therefore because the assessments have generally compiled their inventories on a mass basis and subsequently converted them to an energy, introducing the added variable of specific energy, the per kg results have been the centre of the discussion below.

The results presented exclude end-of-life recycling, although some of the input datasets used in the existing assessments incorporate average recycled fractions.



Figure 6.10 Comparison of battery pack assessments on a mass basis



*Solvent refers to that used in the electrode manufacturing, see Section 3.4.1 for further details.

Figure 6.11 Comparison of battery pack assessments on an energy basis

The comparison in Figure 6.11 also includes the findings from a report (EPA, 2013), which was published towards the end of this project's timeframe and provided insufficient data to quantify the results on a per kg basis. Similar batteries to those evaluated in this assessment, where considered in the EPA (2013) report. However, much of their data is based on that of Notter, et al. (2010) and Majeau-Bettez, et al. (2011). This seems to have led to some anomalies in the results. For example, the cell/pack assembly is suggested to contribute dramatically more CO_{2e} emissions for the NCM and LFP packs than the LMO, with the value given for the LFP assembly approaching the total given for the LMO pack. The report suggests some of the discrepancies were due to inconsistencies between the data for the chemistries and the assumption that the LMO pack uses a solvent-less manufacturing process. This would fit with the use of the relatively high assembly energies in Majeau-Bettez, et al. (2011), for the NCM and LFP cells, whilst other sources were used for the LMO cells.

The reasoning behind many of the anomalies may result from factors which were not presented due to confidentiality reasons. However, due to insufficient data being available to assess them, comparisons with the EPA (2013) findings were limited.

Several other assessments were also found to provide values for battery production, but were far less comprehensive in terms of their battery LCAs. These have not been
incorporated in Figure 6.10 because of a lack of background data to permit assessment of their findings, unknown/unsuitable chemistries, major known omissions, evaluation of different impact categories and/or significant shared data with the included assessments. For examples Samaras and Meisterling (2008) suggested 12kg CO_{2e}/kg of battery and McManus (2012) reported 4.4 kg CO_{e2}/kg of battery when using water as the electrode solvent. However, the results from Samaras and Meisterling (2008) were estimated by converting the energy requirements from an earlier report, Rydh and Sanden (2005), which is the same source used for the assembly energy in Majeau-Bettez, et al. (2011), and the lithium-ion chemistry analysed is unclear. McManus (2012) used data from Zackrisson, et al. (2010), including the assumptions regarding the solvent, and conducted a streamlined assessment that omitted the specific battery manufacturing impacts which will have biased the results.

The author"s results show significant differences compared to the findings in the existing literature. Figure 6.10 shows the differences ranged from a minimum of one third higher, for the LMO pack relative to the results of Notter, et al. (2010), to nearly 70% lower, for the LFP pack relative to Zackrisson, et al. (2010) results. The main reasons for these discrepancies are discussed below. Further details on, the limitations of the existing assessments and the new inventories derived to help improved the accuracy of this assessment, are given in Chapters 3 and 4 respectively.

Assembly energy

The comparison appears to suggest the results of this assessment are high for the LMO pack and low for the others. However, much of the impacts for the NCM and LFP packs in the existing assessments result from the production energy, which is substantially higher than that used for the reports covering LMO packs, due to differences in the data sources and methodologies (see Section 3.4.1).

The results of the author"s assessment, that aimed to use consistent methodologies for all the cell chemistries, showed only minor divergences in the assembly impacts between the different chemistries, 13% to 15%, see comparison given in Table 6.4. There is a degree of ambiguity between what is included in the assembly impacts (see discussion in Section 4.3.5) and what the data refers to. This was a particular problem for the method used in the existing NCM and LPF assessments, which approximated the assembly energy based on existing lumped data, compared to the specific evaluation of battery assembly operations as in this and the existing LMO assessments. For example the lumped data made it unclear

as to what battery chemistries, sizes, volumes or potentially other products the data encompassed and whether associated requirements, such as those for heating/lighting or research/administration operations, were included.

Assessment and lithium-ion	Absolute results	Relative results
chemistry	(kg CO _{2e} / kg of pack)	(% of total pack impacts)
Authors assessment LMO	1.2	15
Dunn, et al. (2012a) LMO	0.3 (calculated)	<6
Authors assessment NCM	1.2	13
Majeau-Bettez, et al. (2011) NCM	6	27
Authors assessment LFP	1.1	14
Majeau-Bettez, et al. (2011) LFP	6	27
Zackrisson, et al. (2010) LFP		
(water as solvent)	8.2	52

 Table 6.4 Comparison of assembly impacts between assessments

The findings of this assessment indicated far lower assembly impacts than those reported in existing NCM and LFP assessments. They are although not as small as those reported in Dunn, et al. (2012a), which is as expected considering the evaluation of this study, discussed in Section 3.4.1, that indicated potential omissions. These discrepancies would address a significant proportion of all the differences shown in Figure 6.10.

The limitations of the input data used to calculate the assembly requirements in this thesis, especially that of the electricity used in cathode production, along with potential variations with process changes and the assembly scope, should be noted though.

Cathode production

This assessment showed the complete cathode to be a major contributor, between 27 to 36% of the total pack CO_{2e} emissions, which broadly correlates to that of existing assessments. However, there are some large discrepancies in the absolute values. For example 7.9kg CO_{2e} per kg of battery was given for the LFP cathode in Majeau-Bettez, et al. (2011), whereas 2.1kg CO_{2e} /kg was found in this assessment. Much of this higher value was attributed to the polytetrafluoroethylene (PTFE) used as the dispersant/binder, as opposed to the styrene butadiene used in this assessment (see Section 4.4.3) and that of Notter. et al (2010).

Checking of the background data in Majeau-Bettez, et al. (2011), indicated the PTFE was modelled using an Ecoinvent process (labelled as tetrafluoroethylene), which was found to exhibit over $320 \text{kg} \text{CO}_{2e}/\text{kg}$ (for context this is higher than that found for circuit boards and over 25 times higher than primary aluminium). However, data from GaBi suggested only $12 \text{kg} \text{CO}_{2e}$ per kg of PTFE which means the impacts may have been dramatically overestimated.

Coincidentally the Ecoinvent process for PTFE was used as a proxy for the polyvinylidene fluoride (PVDF) binder in Zackrisson, et al. (2010), see Section 3.4.1, which would likewise account for some of their high results. Dunn, et al. (2012a) also assumed PVDF as the binder, but the data set they used suggested far lower impacts <3kg CO_{2e}/kg (Wang, et al. 2012b). This resulted in the binder having little impact on their overall results.

This highlights the importance of even a single background dataset. Further analysis into the production impacts of PTFE/PVDF are needed though to ascertain which values are more representative.

Anode production

The revised anode inventory resulted in the impacts in this assessment, 18-21% of the total pack, being generally greater than those reported elsewhere. This was predominantly due to the new graphite inventory (see Section 4.4.3), derived to help overcome the limitations identified in those employed in existing assessments (see Section 3.4.1), and can have a meaningful bearing on the overall results. For example if the baseline graphite inventory for this assessment was used to substitute that given in Dunn, et al. (2012a), their overall battery CO_{2e} results would increase by over 15%, altering their suggestion of graphite being only a minimal contributor.

Similar absolute values for the complete anode were reported in Majeau-Bettez, et al. (2011), but these were found to have resulted from the PTFE binder, as discussed above for cathode production, which contributed over 50% of their value.

The case study of graphite used as the anode active material shows the large discrepancies that could result from the use of proxies for similar materials used in other applications. This is due to the additional processing required for some specialist battery materials (e.g. battery anode graphite verses baked carbon used in the aluminium industry), which could lead to their impacts being substantially greater.

6.6.2. Lithium impacts

The Li₂CO₃, used as the lithium source in the cathode and electrolyte, was found to contribute between 1.3% and 2.2% of the total impacts, for the LFP and NCM packs respectively. Using the values given in Stamp, et al. (2012), for Li₂CO₃ production from ores instead of brine, showed this alteration had little effect on the overall results, which was in line with their findings. This indicated that the supply of lithium is only a fairly small contributor to the total battery impacts; at least when using current sources see Section 4.4.4.

The actual amount of CO_{2e} attributed to the Li₂CO₃, per kg of battery for this assessment, was however considerably higher, approximately 50% for the LMO pack compared to that found in Stamp, et al. (2012). This was due to the larger amount of Li₂CO₃ found to be necessitated in this assessment. Considering the relatively small impacts of the baseline Li₂CO₃ production on the complete battery this was not that significant. However for unfavourable Li₂CO₃ production conditions, in line with those in Stamp, et al. (2012), this resulted in considerable larger quantities of emissions being found in this assessment. For example the Li₂CO₃ was found to contribute approximately 4.8kg CO_{2e} per kg of LMO battery pack for brine unfavourable conditions, which would substantially increase the total pack impacts.

6.6.3. Comparison of recycling impacts

Section 6.5 showed that this assessment found benefits for recycling. However they are far less than those suggested elsewhere which, in some cases, have indicated reductions of over 50% (Dewulf, et al. 2010; Dunn, et al. 2012a; Gaines, et al. 2011).

The recycling benefits given in Dunn, et al. (2012a) mainly resulted from the recycling of aluminium, which is modelled as constituting 19% of the pack mass and over 40% of the total CO_{2e} impacts. When coupled with the low overall findings of this assessment, these benefits indicated a high recycling reduction, up to over 50% in CO_{2e} emissions. The assessment only addressed the materials that potentially have significant recycling benefits. Dewulf, et al. (2010) showed considerable benefits for recycling the cathode material on an energy basis (51%), but also did not consider the other battery materials. The assessment conducted in this thesis addressed all the constituents, some of which were found to possibly incur net impacts e.g. manganese, graphite and the electrolyte.

Gaines, et al. (2011) appear to consider the entire pack and also show reasonably high benefits for recycling, approximately 30% in energy. However they only include the requirements to reprocess the materials, i.e. excluding those of stripping/separating them from the battery, and substances for which no recycling data was available were assumed to be reclaimed with a 50% energy saving. These assumptions are expected to have resulted in an overestimation of the benefits, particularly for current recycling processes.

The EPA (2013) LCA indicated CO_{2e} recycling benefits of around 20%, which are far closer to those found in Section 6.5, and the assessment states that they assumed an optimistic scenario for recycling along with additional work being needed to better quantify the benefits.

Lower benefits for the processing of a complete pack would appear to be justifiable, given the considerations above involving existing assessments of battery recycling. It has also been suggested that recycled lithium currently costs more than primary (Howes, 2012), and that battery recycling economics are highly dependent on the value of cobalt (Georgi-Maschler, et al. 2012). These economic considerations would also seem to indicate processing of whole lithium-ion packs, particularly with little or no cobalt, may be closer to the low values found in this thesis, notwithstanding the limitations given in Section 6.5.

6.7. Additional impact categories

To provide an indication of how the findings may alter between different factors, results for a selection of additional common impact categories are given in this section. Due to global warming potential being the focus when compiling the inventory and the reasons discussed in Section 4.3.3, a higher degree of uncertainty in these results is expected.

In all cases (excluding primary energy) the CML calculation methodologies available within GaBi (see Section 4.3.3) were used. The categories presented are listed below and further details on their derivation and effects can be found in Baitz, et al. (2011).

- Primary energy demand from renewable and non-renewable resources (net value).
- Acidification potential Increased acidification can cause nutrients to be lost from soils and acid rain leading to corrosion for example.
- Ozone depletion potential.

The results are given in Figures 6.12 to 6.14.



Figure 6.12 Results for primary energy demand per kg of battery pack



Figure 6.13 Results for acidification potential per kg of battery pack

Figures 6.12 and 6.13 show that the results for primary energy and acidification potential, without the EoL phase, exhibit trends between the chemistries similar to those found for global warming potential (i.e. the NCM pack has the highest impacts and the LFP and LMO packs have close values).



Figure 6.14 Results for ozone depletion potential per kg of battery pack

The benefits of recycling on acidification potential are shown to be much greater than those for CO_{2e} emissions and result in the NCM pack switching from the highest, to the lowest contender, depending upon whether or not they are included. This phenomenon resulted from the acidification potential being strongly dependent on the metals in the packs, which are mostly recovered in the recycling process. Nickel recycling was found to be a major contributor and accounted for much of the large benefits shown for the NCM pack.

The results for ozone depletion potential, Figure 6.14, show different relative findings amongst the chemistries than those for global warming potential, with the LMO pack exhibiting the highest impacts, and the NCM the least. The increase shown for the LFP pack, incorporating the EoL phase, was found to result mainly from the effects of the steel pack recycling. These were not offset by gains from the cell materials as in the other two packs. Interrogation of the model revealed that the majority of the higher LMO pack value resulted from a process for heat energy from natural gas, included in the Ecoinvent dataset used to model the final LiMn₂O₄ synthesis from the precursors, see Section 4.4.4. Substituting this for a similar process resulted in the LMO pack's ozone depletion potential dropping by about 17%, but negligible impacts on the CO_{2e} findings.

This indicated the highly subjective nature of many impact categories, to even seemingly minor assumptions, and the important variations that can exist amongst datasets that model similar processes.

6.8. Summary

The review of the existing assessment showed relatively high impacts for NCM and LFP packs and far lower values for LMO ones. The results of this thesis however showed little difference between the chemistries and that all the results, although nearer the lower values reported for LMO packs, still differed by minimum of 33% compared to the closest value in the main existing assessments.

Two main causes of differences between assessments were, the assumptions regarding the binder/solvent used during the electrode manufacture, and the assembly energy. In the case of the binder/solvent a large portion of the differences was found to result from the extremely high impacts of the dataset used to model one material, PTFE. Data from a different source however revealed far lower impacts for this material, less than 4% in CO_{2e} terms. If this is nearer the actual value it would substantially reduce the overall findings of some existing assessments. To give an example of the potential importance of this, the CO_{2e} impacts of the PTFE in Majeau-Bettez, et al. (2011) were found to on their own be higher than the values for the entire battery pack in some other assessments.

In terms of the assembly impacts only (see Section 4.3.5) this assessment found minimal differences amongst the three lithium-ion battery variants assessed. Compared to the findings of existing assessments that have evaluated NCM and LFP packs the values were found to be much lower. These assessments utilised assembly energies based on lumped estimations from other sources, whereas this assessment evaluated the requirements at the process-level (i.e. it quantify the requirements of each individual process involved). This was the same approach as was used by Dunn, et al. (2012a), who also noted they attained far lower impacts, to the extent that they were significantly below those of even this assessment. However, this approach requires the evaluation of many processes, estimates or simplifications, which can easily lead to omissions and thus underestimations. Considering the discussion in Section 3.4.1, this could explain why the results of Dunn, et al. (2012a) are substantially below those found here. Some underestimations, compared to other assessments, may also have occurred in the Author"s model. For example due to the scope not specifically including the impacts of lighting and heating the facilities used during battery assembly. These factors may not be directly involved in the battery assembly, but result from it being performed, and will act to increase the values.

The assumptions and inventory used to model anode graphite production were shown to have a notable effect on the results, with the impacts found in this assessment being substantially higher than those in other battery LCAs. These impacts could account for some of the lower values reported in the existing assessments of LMO packs.

The example of graphite acted as a good case study to show the potential effects the data used for a single material, amid an important one in lithium-ion batteries with graphite anodes, can have. Inventory data for battery graphite along with many other specialist materials/processes is limited. This has led to much of the same data/assumptions being used amongst existing battery LCAs and often its prior use being used as its justification for use in subsequent assessments. However the discrepancies found for graphite, along with those for the assembly energy and potentially the PTFE binder discussed earlier, reveal that this could be leading to uncertainty propagation. This reaffirms the importance of checking input data/assumptions, even if consistent with existing assessments, and indicates caution should be observed when verifying results against others.

The inclusion of the EoL phase, which partially utilised primary industrial data, showed benefits in CO_{2e} terms, although substantially lower than often suggested in the current literature.

Overall the findings highlighted several factors whose assumptions can have notable effects on the results and that care is needed to ensure that not only the input assumptions used, but also that the background inventories, are reasonable and representative. This is especially true for processes or materials that are less common in general LCAs, such as the battery active materials. Some LCI data may exist for these but caution should be observed and, if suspected of having a bearing on the results, data must be interrogated to ensure it is reasonable, thereby helping to reduce uncertainty propagation.

Despite the limitations/uncertainties that still surround the model and results derived in this thesis, it builds on the findings in the existing literature providing notable improvements and quantification of the causes of discrepancies.

7. WHOLE VEHICLE MODEL RESULTS AND DISCUSSION

7.1. Introduction

This chapter assesses the CO_{2e} impacts in the context of the whole life of a battery electric vehicle (BEV), building on the results and discussion for the battery model. This was achieved using the whole life vehicle model, with the battery LCA incorporated, as described in Chapter 5. The same limitations discussed in Section 6.2 should therefore be appreciated when interpreting the results.

The findings of this Chapter addressed objectives 4 to 6 of the project and part of 7 (Section 1.4.5). Specifically these were the effects of the battery life cycle, parameters and trade-offs on the whole vehicle, along with comparisons against a conventional powertrain.

Comparisons of electric and conventional vehicles have been presented numerous times in the existing literature (e.g. Notter, et al. 2010; Ma, et al. 2012; Hawkins, et al. 2013). However the findings are very sensitive to assumptions, such as the electricity used to charge the BEVs (Section 2.1.4), the parameters of the comparison vehicles (Section 2.2.3) and the technology/efficiency level which is improving with time (Section 3.3.1). These factors are in addition to those arising from the battery itself and complicate comparisons with other assessments at the vehicle level, because it is often unclear as to where differences arise. For example they may be due to differences in the battery impacts or from discrepancies in the vehicle parameters.

This assessment has included a comparison conventional vehicle. However the main contribution of this thesis concerned quantifying the hitherto inexplicitly documented impacts and effects of vehicle batteries. Due to this, and the considerations above, only cursory discussion of the absolute impacts of BEVs relative to conventional vehicles is given.

The first section of this chapter employs the use phase model to identify the changes in vehicle in-use energy consumption resulting from differences in the batteries. Following this, the baseline results for the whole vehicle simulations are reviewed and the effects of the different battery options contrasted. The impacts of variations in battery performances, production/EoL inventories and the use phase are then investigated. Finally the main findings are summarised.

7.2. Vehicle requirements

Iterations of the use phase model were run to establish the battery pack mass needed for each of the lithium-ion chemistries assessed, i.e. lithium manganese oxide (LMO), lithium iron phosphate (LFP) and nickel cobalt manganese (NCM), in order to achieve the range of 175km defined in the Functional unit (see Section 5.3.1). The model was then used to identify the vehicle energy requirements at different stages, the results for which over the New European Driving Cycle (NEDC) and using the baseline assumptions (see Table 5.5 and Table 7.1), are presented in Table 7.2.

Factor/variable	Baseline value
Cell mass percentage of total pack	60%
Pack specific energy for 60% cell mass (values in	LMO 91.8Wh/kg (153)
parentheses refer to cell level specific energy)	NCM 122Wh/kg (204)
	LFP 84.6Wh/kg (141)
Pack capacity fraction used	80%
Resistance multiple	1
Static charging/battery system efficiency (excluding	85%
battery resistance)	

Table 7.1 Baseline assumptions for battery and use phase parameters

In Table 7.2 the usable energy supplied refers only to the battery output, i.e. the energy usable by the motor/inverter or auxiliaries. The value for energy supplied from the grid also includes all the losses between the grid connection and final battery output, whose default efficiency was taken as 85%, plus any additional losses resulting from the battery resistance model which varied with power demand, SOC and cell type (see Sections 5.8.2 and 5.8.3).

	Cell type used in pack		
	LMO	NCM	LFP
Battery mass needed for 175km range (kg)	319	236	353
Usable energy supplied by battery (Wh/km)	135	131	136
Energy supplied from grid (Wh/km)	162	157	163
Percentage change in energy supplied from grid	0	-3.1	+0.6
relative to LMO (%)			

Table 7.2 Calculated battery mass and in-use energy requirements

Table 7.2 shows that the pack using the LFP cells would be 117kg heavier than one using the NCM cells to attain the fixed BEV range of 175km. This higher mass, along with lesser effects from the battery model, resulted in the vehicle simulated with the LFP pack consuming nearly 4% more energy during the in-use phase, relative to one incorporating the NCM pack. In comparison to the LMO pack there were still distinct benefits for the NCM pack, but marginal penalties for the LFP.

The figures showed that over the NEDC the resistance model (see Section 5.8.3) predicted efficiencies of 97% to 98%, for all the cell types. These fell within the range reported by Omar, et al. (2012), but are higher than those found in, for example Mulder, et al. (2013), and the fixed assumptions used in many other assessments (e.g. Campanari, et al. 2009; Gerssen-Gondelach, and Faaij, 2012). However, the model only accounted for losses from the battery resistance and the power demands over the NEDC are relatively low considering the pack size. The low power demands will have acted to improve the efficiency of the variable model used in this assessment, as shown in Section 5.8.3, which could explain much of the discrepancy against cell test results such as those presented in Mulder, et al. (2013) which use more demanding cycles. This effect resulted in the simulated efficiency over the adapted driving cycle, see following section, more closely matching those of other assessments. Additional factors such as temperature, depth of discharge and potential losses due to cell balancing will also affect the results. Further work is needed to more extensively validate the battery resistance and charging/battery system efficiency models.

Altering the fixed portion of the battery/charging system efficiency (see Sections 5.8.2) between 80% and 90%, resulted in approximately a 6% increase and 5% decrease respectively, in the energy supplied from the grid. This shows that improvements in the battery/charging system could enable significant gains.

Vehicle range was set in this thesis to equalise vehicle utility in battery comparisons. However simulations, which are presented in Sweeting, et al. (2011), were performed to show the effects of battery specific energy, and thus mass, on vehicle range. These showed a scenario of diminishing increases in range for larger battery packs, which became more acute as the battery specific energy was decreased. Battery specific energy is thus not only a vital factor in the efficiency of BEVs, but also in their practical range and thus utility.

7.2.1. Effects of use phase assumptions

The results of applying the adapted driving cycle, used to provide an indication of how real-world usage may affect the results (see Section 5.8.5) and assuming no alterations to the battery pack mass, are given in Table 7.3. This shows the difference between the in-use energy consumption has increased to nearly 6% between the NCM and LFP packs, see Figure 7.1.

	Cell type used in pack		
	LMO	NCM	LFP
Battery mass used (kg)	319	236	353
Usable energy supplied by battery (Wh/km)	178	172	181
Energy supplied from grid (Wh/km)	219	208	220

Table 7.3 In-use energy requirements for adapted driving cycle



Adapted driving cycle with increased battery resistance

- Results over adapted driving cycle
- NEDC with increased battery resistance
- Baseline results over NEDC

Figure 7.1 Impacts of variables on in-use energy consumption

The higher power demands in these simulations resulted in a decrease in the battery efficiency of 2% for the LMO pack, which falls within the range reported in Smith and Wang, (2006). This meant that, although the energy requirement from the grid was increased by 35% relative to that over the NEDC (see Section 5.8.5), the usable energy supplied by the batteries only increased by 32%. A lower reduction was found for the NCM and LFP packs, approximately a 1% battery efficiency drop. This, coupled with the

differing masses, resulted in the total energy consumption increase for the adapted driving cycle differing, with only 32% (opposed to 35% for the LMO pack) found in the case of the NCM pack. The data used to construct the battery models was based on large cells similar to those anticipated to be used in BEVs. However alternative cells may have different charge/discharge profiles and resistances, which will affect the results.

To study the effects on the model and to simulate some of the possible effects of aging on the cell, the battery internal resistance was doubled (see Section 5.8.3 and Figure 7.1). Over the NEDC this resulted in an increase in energy consumption of approximately 1% for all the packs. However, greater increases and variations amongst the packs were found over the adapted driving cycle due to decreases in the battery efficiency. The maximum increase was approximately 3% for the LMO pack. This resulted in the 35% increase in energy for the adapted driving cycle, rising to approximately 40% relative to the baseline.

The findings showed that the differences amongst the battery efficiency models for the three packs have small effects over the baseline NEDC simulations. However, over more demanding cycles, such as those often experienced in the real-world, they may increase significantly which also leads to an amplification of the cell aging effects.

7.3. Life cycle effects of the battery on the whole vehicle

The findings of the combined vehicle and battery models are presented in the following sections, which show the effects of the battery on the lifecycle of a BEV. This section addresses the baseline results and those that follow assess the influences of some of the key variables.

7.3.1. Baseline results

Figure 7.2 shows the results over the NEDC using the values given in Table 7.1 and a lifetime distance of 150,000km (see Section 5.3.1). GaBi data for the EU27 grid mix as consumed by private households, which exhibited impacts of $485g \text{ CO}_{2e}/\text{kWh}$, was used to model the in-use electricity.



Figure 7.2 Whole life vehicle impacts including recycling

Regulations dictate that EoL processing and recycling of vehicles and batteries is performed (Council Directive 2000/53/EC; Council Directive 2006/66/EC). The impacts of EoL processing and credits for reclaimed materials have therefore been incorporated in the baseline results for the whole vehicle, as in Figure 7.2. Results, for the assumption that no recycling was performed, showed only slight increases from the battery impacts, as would be expected from the modest recycling benefits shown in Section 6.5. Overall excluding recycling caused an increase of between 5% and 6% in the BEV CO_{2e} emissions shown in Figure 7.2, mainly due to the lost benefits from recycling the rest of the vehicle.

The figure shows little difference between the BEVs with the LMO and LFP packs, approximately 1%. However the vehicle fitted with the NCM pack showed larger differences, with approximate reductions of 5% and 6% relative to those using the LMO and LFP packs respectively. These reductions were found to result mainly from the battery manufacturing impacts, over 60%, whilst the use phase contributed the remainder. The model however did not account for any secondary changes to other components due to mass savings, which could increase the in-use benefits of lighter battery packs, such as alterations to the motor to help ensure it runs at the same efficiency points or reductions in structural components due to lower loads.

Both the manufacturing and use phase benefits of the NCM pack were linked to the higher specific energy of this cell type, without which the impacts would be higher than for the other packs as shown in Figure 6.4. This was due to the lower battery mass needed for a given range and thus reduced production and in-use impacts.

The results for a conventional vehicle were also incorporated. These were based on the manufacturing inventory outlined in Chapter 5, the in-use consumptions of a current efficient diesel vehicle (see Section 5.8.6) and GaBi data for the production/supply of diesel in the EU. However it is only provided to give some context to the BEV results and the caveats discussed in Section 7.1 should be appreciated.

Compared to this comparison vehicle, the BEVs showed relative reductions of between 16% and 21% depending upon the battery pack. This indicates the choice of battery pack could significantly change the relative benefits of BEVs. For example, compared to the conventional vehicle, the CO_{2e} reductions of the BEV using the NCM pack were 30% higher than for one using an LFP pack. The comparison also shows the battery manufacturing impacts result in the BEVs exhibiting substantially higher production values than those of conventional vehicles, nearly 50% when incorporating the LFP pack.

The percentage breakdown for the results is given in Figure 7.3. This shows that under the baseline conditions, factors other than the generation of the in-use energy contribute substantially, over 40%, to the total CO_{2e} impacts of BEVs. The battery packs are a notable contributor at between 10 to 13%. To give some perspective, the absolute values for the battery packs are approximately 1.9 to 2.6 tonnes of CO_{e2} per vehicle. These equate to the tailpipe emissions of driving around 18,000 to 25,000km over the NEDC in the comparison diesel vehicle.



Figure 7.3 Percentage breakdown of overall BEV CO_{2e} impacts from Figure 7.2

7.4. Effects of variables

This section studies the effects of battery variables on the baseline findings. The subsections on driving cycles and in-use electricity sources are more relevant to the use phase of BEVs than their batteries. However, they are very important factors in the whole life emissions of BEVs, and they impact the relative importance, as well as the performance in the case of driving cycles, of their batteries.

7.4.1. Battery lifetime

Battery lifetime is an important parameter and can vary for a variety of reasons, see Section 2.3, which leaves questions as to how long lithium-ion battery packs will last under real-world conditions in BEVs. This creates uncertainty as to whether a battery pack will last the expected lifetime of a car, which is around 13 years on average (Collins, et al. 2002). It is suggested that battery manufacturers are seeking a lifetime of 10 years (Dinger, et al. 2010; EPA, 2013), which would still leave a potential shortfall.

To indicate the effect of the battery lifetime, Figure 7.4 was constructed. This shows the consequences of the battery pack requiring one replacement and the possible influences of cell aging, caused by increased battery resistance see Section 7.2.1.



Including one battery replacement

Baseline results

Figure 7.4 Effects of battery lifetime

The impacts increased by up to 13% with the inclusion of an additional replacement battery pack and the significance of the battery on the total vehicle lifetime escalated to between 18% and 23%.

LFP cells are generally expected to exhibit superior lifetimes, with for example cycle lives of around 2000 cycles reported, compared to 1500 for NCM and 1000+ for LMO cells (Johnson Matthey Battery Systems, 2012). However battery lifetimes are difficult to predict due to variations with in-use conditions and construction, e.g. material purities. Degradation also occurs with age as well as cycling, which considering the relatively long lifetime of vehicles could have a significant affect. The cycle lives given are thus only intended to provide a rough guide of how the batteries assessed compare and the actual values may differ significantly.

The dashed line in Figure 7.4 shows that the LFP pack is still likely to exhibit similar or higher impacts, even allowing for some aging effects in the other cells. If the LFP pack could last the life of a vehicle, whereas the others would require replacement, it could offer benefits. However against the NCM pack they are fairly modest. Considering this, if the use of two NCM battery packs could enable an increase in the lifetime distance, they may again offer benefits over LFP packs attaining the baseline 150,000km. This effect is assessed in the following section.

7.4.2. Vehicle lifetime distance

The vehicle lifetime distance can have a significant impact on the results and is a common source of variation amongst assessments. Figure 7.5 shows the consequences of altering the distance between 100,000km and 250,000km (62,000-155,000 miles) on the findings of this assessment. With current technologies the higher end of this range is anticipated to require a battery replacement; therefore this scenario is also incorporated in the figure.



Figure 7.5 Effects of vehicle lifetime distance

The graph shows how the relative gains decrease for all the scenarios as the lifetime increases, due to the production impacts becoming more dispersed. For example a >4% reduction in CO_{2e} emissions was exhibited for a 10,000km life extension at 100,000km, whilst only 1% was found for the same extension to a 240,000km life. This resulted in the impacts, for the vehicle with the LMO pack, increasing by 19% if the lifetime was abated to 100,000km, but only decreasing by 9% when it was increased to 200,000km. These results however are subjective to the use phase emissions, for example differences in the grid impacts used to charge the vehicles.

Figure 7.5 also reveals that there may only be a limited window where the LMO or LFP packs could offer CO_{2e} benefits over NCM ones in a BEV. The baseline values in this assessment suggested that an increase in lifetime distance of approximately 30,000km or 20%, relative to the 150,000 km base, would be needed for the LFP pack to offer benefits over the NCM. However, if a vehicle was fitted with a replacement NCM pack it would only need to extend the range beyond 164,000km, to offer gains over one attaining the baseline 150,000km with a single LFP pack.

The assessment has also only considered whole battery packs, with all the burdens being attributed to the first life, i.e. the vehicle they were fitted to when new. If for example a replacement NCM pack could be reused to enable a second vehicle to reach EoL, the impacts could approximately be halved between each vehicle. This would bring the values shown in Figure 7.5, for the NCM pack with replacement, down to just below those shown for the LMO pack without replacement.

7.4.3. Battery pack parameters

Chapter 6 analysed the effects of some of the key assumptions used in the battery LCA model at the battery level. The subsections below build on this by looking at their influences on the whole life of a BEV.

Cell mass fraction

During alterations to the cell mass fraction, the cell specific energy was assumed to remain constant; therefore it altered at the pack level (see Section 6.4.2). For the LMO pack, and 50% to 80% cell mass fraction, the pack specific energy varied between 77 and 122Wh/kg. To account for these changes the use phase model was re-run to establish the required battery mass and corresponding vehicle consumptions, as in Section 7.2. The results

presented in Figure 7.6, for the cell mass fraction, therefore also provide an indication of the approximate effects of changes in the specific energy.



Figure 7.6 Effects of cell mass fraction on vehicle CO_{2e} emissions for LMO pack

Figure 7.6 shows that when the cells are decreased to 50% of the pack mass, the impacts increase by approximately 3%, and when they are increased to 80%, they cause a 4% decrease, relative to the baseline results. Removing the effects of changes in the battery production impacts with cell fraction caused the variations to increase to approximately +4% and -5%, respectively. This effectively showed the impact variations resulting just from changes in the specific energy. These were +4% for a 17% decrease in specific energy and -5% for a 33% increase; which showed improvements in the battery specific energy can have a notable effect on the whole vehicle. However, the lower results found in the figure indicate part of the benefits are likely to be eroded by increases in the production impacts and fairly large improvements are needed to make substantial differences.

Overview of battery effects

The vehicle lifetime findings for some of the main battery variables are presented in Table 7.4. Results are given in terms of both the percentage change in the vehicle CO_{2e} emissions and the actual lifetime mass alteration, relative to the baseline BEV with the LMO pack. The results for a ±10% change, in the baseline battery impacts, are also given to provide an indication of the effects of a major change to an important factor, such as the inventory for the cathode active material, see Section 6.3.1.

Approximately 40% of the variations for the cell mass fraction changes resulted from the in-use phase, whereas that for the other factors emanated solely from the battery production/EoL impacts.

Variable factor	% change in lifetime	Total lifetime change
	vehicle CO _{2e} emissions	in emissions (kg CO _{2e})
Cell mass fraction +10% (70% cell	-2.2	-440
mass)		
Cell mass fraction -10% (50% cell	+3.2	+650
mass)		
Anode artificial graphite produced	-0.5	-92
using hydroelectricity		
Anode natural graphite from China	-0.8	-162
Removal of battery recycling	+0.3	+65
benefits		
Battery recycling with manganese	-0.5	-96
and graphite sent to landfill		
50% increase in BMS circuit board	+0.7	+137
mass		
50% decrease in BMS circuit board	-0.7	-137
mass		
10% increase in battery impacts	1.2	249
10% decrease in battery impacts	-1.2	-249

Table 7.4 Effects of battery variables relative to baseline LMO pack

Table 7.4 indicates that many of the battery variables discussed in Chapter 6 only have marginal effects at the vehicle level; nevertheless the cumulative absolute impacts at the fleet level would be very significant. Combinations of the effects in Table 7.4 could conspire to alter the vehicle lifetime impacts by around +5%, assuming a worst case for all the factors listed, and by -5% for a best case. Considering the modest reduction shown for the BEV, compared to the conventional vehicle in Section 7.3.1, even the small variations shown could alter this benefit by a relatively significant proportion.

Vehicles have fairly large impacts associated with their lifecycles, approximately 20 tonnes of CO_{2e} emissions for the baseline BEV, which masks the absolute effects of some of the changes. For example, in absolute terms, the minimum change in Table 7.4 is 65kg of CO_{2e} emissions. This, although small in comparison, is still equivalent to the tailpipe emissions of travelling more than 600km in the conventional comparison diesel vehicle over the NEDC and would be substantial at the fleet level.

7.4.4. Vehicle use phase

The impacts of the adapted driving cycle, used to provide an indication of possible realworld usage, on the whole vehicle life are presented in Figure 7.7.



Figure 7.7 Comparison of whole life vehicle impacts over adapted driving cycle

This showed that the results increased by between 19% and 21%, compared to those simulated over the NEDC. This eroded the relative impacts of the battery on the whole life, because all the increase occurred in the use phase. Compared to Figure 7.3, the findings of Figure 7.8 show their overall significance drops by 2%, to a minimum of 8%.



Figure 7.8 Percentage breakdown of overall impacts over adapted driving cycle

The greater impacts of the use phase, together with the escalated deviations amongst the vehicles with the different batteries (see Section 7.2), will impact on the findings reported for variations in the battery and vehicle lifetimes (see Sections 7.4.1 and 7.4.2). Figure 7.9 presents the same results as Figure 7.5, but for the adapted driving cycle. This shows that the benefits of the NCM pack are nearly sufficient to absorb the impacts of a battery replacement for the baseline distance, and may even drop below those for a vehicle with one LFP pack above 200,000km.



Figure 7.9 Effects of vehicle lifetime distance for adapted driving cycle

Increasing the lifetime distance acts to further decrease the batteries significance, on top of that found for the adapted driving cycle. However, even for the case of its least significance, 250,000km lifetime and one NCM pack, the battery still represents approximately 6% of the total vehicle lifetime CO_{2e} emissions.

The effects of the adapted driving cycle on the variations due to battery factors, given in Table 7.4 which were not dependent on the use phase, was to reduce the percentages by approximately one sixth, although the absolute lifetime changes remained unaltered. For the cell mass fraction the use phase variations acted to abate this reduction.

7.4.5. Electricity generation

The importance of the electricity source used for charging electric vehicles, and the associated problems, were introduced in Section 2.1.4. The results for some alternative grids and common generation sources are given in Figure 7.10 to indicate the variability.

The data was taken from GaBi 6 with the values for various generation sources being based on UK data. However, they will vary for reasons such as spatial and technological differences. For example published estimates for wind generation range between 1.7 and $81g CO_{2e}/kWh$ (Dolan and Heath, 2012).



Figure 7.10 Emissions associated with various electricity sources

Figure 7.10 indicates the baseline value used in this assessment, EU grid mix, sits around the middle of the range (excluding India's grid) and is similar to generation using natural gas exclusively. The higher value reported for India's grid, compared to coal generation which refers to the UK case, results from differences in the grid/generation plant - especially that from the large transmission and distribution losses associated with India's grid (Defra, 2012).

The emissions range is vast, approximately two orders of magnitude. Therefore to encapsulate this, simulations were conducted for grid emission intensities ranging from virtually zero up to 1.5kg CO_{2e}/kWh. This should indicate the best and worst cases for electricity generation, the results of which are presented in Figure 7.11 for a vehicle using the LMO battery pack, together with those for an efficient conventional diesel vehicle (Section 5.8.6).



Figure 7.11 Effects of in-use electricity grid emissions for vehicle with LMO pack

Figure 7.11 shows that the results presented for the baseline case could be approximately halved, using low emissions grids such as in France, or even more so using low carbon sources such as wind and hydro. At the other extreme, they are more than doubled when using very high emissions grids such as in India. However as mentioned above India"s grid emissions are huge even compared to many coal power plants.

The effects of changing the in-use electricity emissions on the relative importance of the battery, on the vehicle lifetime impacts, are also indicated. This shows that the battery pack could represent approaching 30% of the lifetime CO_{2e} impacts, if very low emission in-use electricity was used. The proportion drops as the grid emissions increase, but even for the worst case, the LMO battery production still represents about 5% of the lifetime impacts of a BEV. Due to the lower impacts, found for the NCM battery pack (Figure 7.8), the combination of very high use phase grid emissions and the adapted driving cycle were found to result in a lower minimum battery significance of approximately 3.5%. However, the values for the NCM pack exceed 5% for electricity sources below 950g CO_{2e} /kWh, which is not far off that shown for pure coal generation in the UK (Figure 7.10).

The battery production impacts in Figure 7.11 were assumed to remain fixed, while those of the in-use phase changed according to the electricity emissions. However, changes in grid emissions will also affect the battery production impacts. Spatial and temporal differences are therefore likely to affect both the production and use phases, e.g. the battery LCA referred to average production in Europe and different findings are likely to be attained if this were to alter. This is expected to reduce the changes shown in the battery

impact significance, meaning the deviation from the baseline will decrease. For example, most electricity grid emissions are reducing with time and future reductions are envisaged (Hawkes, 2010; DECC, 2011; Defra, 2012). This will abate the production, as well as the use phase impacts and thus reduce the relative increase in the battery significance shown in Figure 7.11. The reverse should occur for increased grid emissions. Considering this, and the very high grid emissions on the right-hand side of Figure 7.11, indicates that based on the results of this assessment, a minimum battery lifetime CO_{2e} emissions significance of 5% is likely to be a low value, even in the case of the NCM pack.

Figure 7.11 can also be used to investigate the effects of marginal electricity, which was discussed in Section 2.1.4. For example, if the marginal electricity emission factor, reported for the British grid between 2002 and 2009 (690 g CO₂/kWh) in Hawkes (2010) was used, the total vehicle impacts would increase by about a quarter over those of the baselines.

The crossover electricity emissions, where the impacts of the BEV equal those of a comparison vehicle, can be calculated using equation (7.1).

Crossover electricity emissions
$$g CO_{2e}/kWh = (E_{CV}-E_{BEVP})/C_{BEV}$$
 (7.1)

Where:

 E_{CV} = The whole life emissions from the vehicle a BEV would substitute (g CO_{2e} per km).

 E_{BEVP} = The BEV emissions excluding those of the in-use electricity, i.e. those of the battery, glider and maintenance (g CO_{2e}/km).

 C_{BEV} = The electricity consumption of the BEV in kWh per km.

This gave crossover electricity grid emissions of approximately 650 g CO_{2e}/kWh , using the baseline values and the low emission conventional diesel vehicle as shown in Figure 7.11. Sensitivity analysis, of each of the terms in equation (7.1), revealed the whole life emissions for the substitute vehicle (E_{CV}) incurred the greatest variations. For a change of $\pm 20\%$ in the input value of E_{CV} , the crossover emissions varied between 450 and 850 g CO_{2e}/kWh . Variations in the battery pack production impacts were found to raise the crossover point by approximately 1.5% for every 10% reduction in their value and vice-versa.

Uses of low emission electricity

In many geographical areas there are likely to be restrictions on low emission energy sources e.g. cost, availability and practicality (see Section 1.2.1). This raised the question of what is the best use of limited new low emissions electricity capacity, see Section 2.1.4. The crossover point, calculated with equation (7.1), is useful for assessing this because it also corresponds to the emissions value, of other potential uses of the same electricity, above which their substitution would offer larger overall gains than BEVs. To illustrate this, Figure 7.12 was constructed. This shows the potential savings of new electricity capacity with emissions ranging up to 800 g CO_{2e}/kWh , used in either a BEV to substitute the assessed diesel vehicle, or to displace coal electricity generation used to meet existing electricity demands with emissions of 1kg CO_{2e}/kWh (Figure 7.10).



Figure 7.12 Optimal use of low emission electricity

Figure 7.12 shows that although the BEV offers emissions savings up until the crossover point, increasing as the emissions of the new generation source used to charge them decrease, they remain less than those attained if existing coal generation could be alternatively substituted. The improvement ratio, also shown and calculated according to equation (7.2), indicates that at the most favourable point for the BEV (i.e. new electricity generation approaching zero emissions), it would only offer 65% of the CO_{2e} reductions attained for substitution of coal grid electricity. However other emissions and factors need to be considered to ensure the optimum overall choices, e.g. BEVs could also help mitigate harmful particulate emissions in urban areas.

Where, providing E_{grid} - E_{NC} is positive:

 E_{NC} = The emissions associated with the new electricity generation (g CO_{2e}/kWh).

 E_{grid} = The emissions from the existing generation that could be replaced (g CO_{2e}/kWh).

The effect shown in Figure 7.12 occurs until the emissions of alternative uses of new cleaner electricity, i.e. existing grid coal generation in the example, drop below the crossover emissions. Past this point a reversal of the effect shown occurs, with the BEV offering greater benefits than the alternative electricity use and the improvement ratio exceeding unity.

7.5. Summary

Many of the battery factors discussed have relatively small influences on the whole vehicle lifetime. However, vehicle manufacturers are actively chasing small improvements and consequent emissions savings in many areas, e.g. mass, aerodynamics and engine performance, such that the cumulative gains become significant at the vehicle level. For example, Mercedes reported a 16% lifetime CO_{2e} emissions reduction for their A class 180 BlueEFFICIENCY (launched in 2012) over their predecessor model. This was the culmination of numerous improvements ranging from engine downsizing and lightweight panels, to low friction wheel bearings and an optimised underbody to reduce drag (Daimler AG, 2012). New generation vehicles that include alternative powertrains are no exception. Any savings, such as those from alterations in the battery production impacts, can be viewed as contributors, helping to meet the overall goal of reduced lifetime impacts.

In line with the rest of this chapter, unless otherwise stated, the impacts and percentage changes discussed below refer to those of CO_{2e} equivalent emissions (see Section 6.2.1).

7.5.1. Whole vehicle results

Little difference was found between the vehicles fitted with the LMO and LFP packs. However the NCM pack showed reductions of 6% relative to the LFP, due to the higher specific energy of this cell type. The fairly substantial mass saving of the NCM pack resulted in over 37% of this reduction coming from the use phase. The remainder was due to the lower battery production impacts incurred by the much lighter pack, i.e. 236kg as opposed to 353kg for the LFP. This finding highlighted the importance of the functional unit. For example if the use phase impacts are assumed to be fixed, as in EPA (2013) and Hawkins, et al. (2013), the benefits of lighter packs, i.e. those with higher specific energies, could be substantially underestimated. Lighter packs reduce the in-use vehicle consumptions, which in-turn reduce the amount of stored energy required for a given range and thus enable further reductions in the battery mass needed. The specification of a range in the functional unit of this assessment, together with the use phase model, enabled these effects to be accounted for. They were found to have reduced the NCM pack mass, and thus production impacts, by approximately a further 4%, compared to a scenario where the in-use energy was assumed to remain constant at that found for the vehicle with the LFP pack. A further consideration that will impact the results between the different batteries is the useable capacity. This was taken as 80% for all the cell types in this assessment, see Section 5.8.3. However this value may alter with battery chemistry and future developments, which will have a similar effect to changing the specific energy, i.e. by altering the pack mass required for a given range.

Compared to an efficient diesel vehicle (see Figure 7.2 and the limitations regarding comparisons in Section 7.1), the baseline BEV values were found to be lower for all the battery types, even when a pack replacement was assumed. The maximum decrease was 21%, but this will alter with factors such as, the emissions of the electricity used to charge the BEVs.

7.5.2. Effects of variables

Battery efficiency

The battery efficiency, modelled on internal resistance, was indicated to have a fairly small impact on the vehicle demands over the NEDC. However the effects became more pronounced for harsher driving regimes. The model indicated around 3% of the increase in the use phase energy consumption, found for the adapted driving cycle and LMO battery pack, resulted from decreased battery efficiency rather than increased vehicle demands.

The same trends were found for the possible effects of battery aging. These showed a further 3% increase in the in-use energy consumption over the adapted driving cycle, which equated to just over a 2% increase in vehicle lifetime CO_{2e} emissions if this effect was constant throughout a BEVs life. The combination of the adapted driving cycle and

battery aging resulted in approximately 7%, of the simulated use phase energy consumption, being attributed to the battery efficiency resistance model.

This shows that when studying the effects of driving cycles on BEVs, dynamic battery efficiency calculations are needed to account for the total changes, and that as batteries age they will abate the vehicle efficiency.

Real-world driving cycles

Due to the other phases of the vehicle"s lifetime, the large real-world in-use increases found, 35% see Section 5.8.5, reduced to an approximate 20% CO_{2e} rise at the whole vehicle lifecycle level, relative to those over the NEDC. This is still a substantial increase and acted to reduce the apparent significance of the other phases.

Lifetimes

Investigation into the battery and vehicle lifetime showed that the necessity for a battery replacement had a significant impact on the overall baseline CO_{2e} results, increasing them by up to 13%.

The effects of the assumed lifetime distance were shown to diminish as the distance covered increased. For a $\pm 50\%$ change in the baseline assumption of 150,000km, maximum variations of between $\pm 19\%$ and -9% in the total CO_{2e} emissions were found. However the incorporation of an additional battery pack, to allow the baseline distance to be maintained, was found to reduce the 19% maximum increase, found for a vehicle with a LFP pack and life of 100,000km, to less than 13%.

LFP cells are generally reported to offer higher lifetimes than the other types assessed. However combined studies of lifetime distances and battery replacements for the different packs revealed that, even if they attain substantially greater lifetimes than NCM packs, they would only offer CO_{2e} benefits under a limited set of scenarios. This is due to the lower in-use and production impacts of the lighter NCM packs. For example, using the results for the adapted driving cycle, a vehicle fitted with one NCM pack would need a lifetime of less than 121,000km before one using an LFP pack and attaining the baseline distance would offer benefits. However, if the vehicle with the NCM pack were to have the battery replaced it would only need to extend the range to over 155,000km, i.e. a 5000km increase assuming the vehicle with one LFP pack only attained the baseline distance, to again offer lower emissions. Furthermore if partial pack substitutions are possible the CO_{2e} benefits of using LFP packs with longer lives may also be abated under these scenarios.

When selecting a battery pack for a BEV there will be trade-offs between specific energy and lifetime. From the results, the increased energy offered by NCM cells appears to offer greater benefits under many scenarios than fairly substantial changes in lifetime. However, this assessment has been predominately confined to CO_{2e} impacts and the use of two NCM battery packs for example may result in more resource depletion than one LFP pack.

Electricity generation

The electricity grid emissions were shown to not only have a major effect on the vehicle impacts, but also on the relative significance of the battery and the differences found for the adapted driving cycle. Using low emission electricity sources to charge BEVs resulted in their potential CO_{2e} benefits increasing to over 60%, relative to the conventional diesel vehicle.

Low emission electricity capacity is presently limited in many geographical areas. Subsequently other potential uses were investigated to help identify whether BEVs represent the most appropriate use of this energy. This showed that the crossover electricity grid emissions, i.e. the level at which the impacts of a BEV equal those of the vehicle it could substitute, also represent the level from alternative uses above which their substitution would offer greater benefits. An example indicated that, although the use of low emission electricity to charge BEVs would offer CO_{2e} benefits, if coal or other high emission sources used to meet existing demands could instead be displaced by the same electricity, larger overall gains may be achieved. However, this takes no account of other emissions/benefits or the proposed effects of vehicle-to-grid systems offered by BEVs, such as damping of the variation from renewable generation (Peterson, et al. 2010).

Battery pack production parameters

None of the main battery production variables assessed were shown to have large impacts relative to the CO_{2e} emissions at the whole vehicle level. At the fleet level the absolute savings or detriments would be large though, as discussed above.

The reasonably small alterations mean that deviations from the assumptions, used in the battery LCA model constructed in this thesis, should only have fairly small impacts on the findings at the vehicle level.

Increases in cell specific energy were found to be beneficial, but there are trade-offs with production impacts. For example a 10% increase in the LMO cell specific energy was found to offer lifetime benefits, providing it did not increase the battery production impacts by more than 15% on a mass basis.

7.5.3. Battery significance on the whole vehicle

The baseline results, and those for the adapted driving cycle, showed that the production/EoL phases of all of the battery packs assessed represented around 10% of the whole life BEV CO_{2e} emissions. Variations in the assumptions used in the battery LCA had little effect on these findings.

Changes in the use phase grid emissions and battery/vehicle lifetime were found to have a significant impact. However, the battery impacts did not drop below 5% of the total vehicle lifetimes, unless extremely adverse conditions were employed, such as using purely coal electricity generation to charge a BEV fitted with the lowest impact battery pack and operated over the adapted driving cycle. Conversely, factors such as the necessity for a battery replacement or use of low emission in-use electricity could substantially increase the significance.

Overall a value of approximately 10% would appear to be a good estimation of the significance of lithium-ion batteries on the whole life CO_{2e} emissions of BEVs, given current or near future technologies.

The research findings therefore indicate that the batteries of electric vehicles are notable contributors to their impacts and need to be considered in sustainability assessments. Together with the rest of the vehicle, the battery impacts meant the production/EoL phases could already represent around 40% of the lifetime CO_{2e} impacts and with improvements to grid emissions this is likely to increase.

8. CONCLUSIONS, OUTLINE FRAMEWORK AND RECOMMENDATIONS FOR FURTHER WORK

8.1. Introduction

Light duty vehicles (LDV) are a vital source of mobility for many and interlinked with global economies. Various alternative powertrain and fuel options have been proposed to help alleviate the problems associated with these vehicles. Out of these, battery electric vehicles (BEVs) have been identified as currently offering the greatest potential to minimise energy consumption and emissions during their usage. However several challenges face BEVs including range, cost and electricity grid emissions. Some of these factors have received considerable attention, but literature data on the production and end-of-life (EoL) impacts of their large battery packs is limited and highly variable. This variability can have a significant impact on whole life assessments of BEVs.

To help resolve this uncertainty, and provide an enhanced understanding of battery variables on whole life vehicle impacts, an holistic life cycle assessment (LCA) of BEVs focusing on lithium-ion traction batteries was developed.

The key research conclusions, presented in Section 8.2, were utilised to derive an outline framework for assessing the sustainability of advanced powertrains (see Section 8.3). The final sections (8.4 and 8.5) summarise the main novel contributions and important areas that would benefit from further research.

8.2. Overview of research findings

The research generated significant improvements concerning sustainability assessments of BEVs, see Section 8.4. These were achieved through the development of enhanced models for the production, EoL and use of BEVs which enable the main findings given below to be concluded. Further details are given in the project methodology outlined in Section 1.6. However the number of variables involved, data limitations and rate of technological change mean there is still a degree of uncertainty in the findings and that on-going research is required.

8.2.1. Overall findings

Incorporation of representative battery production and EoL impacts are vital in sustainability assessments of BEVs, to assess their true effects and enable effective

comparisons with other powertrains. Without their inclusion, significant changes in the relative differences between alternative powertrains may be found. Lifetime emissions benefits can be achieved through the selection of optimal battery types for use in BEVs, even amongst variants of lithium-ion cells. However there are trade-offs between factors.

These high level conclusions resulted from the findings of the many variables related to BEVs evaluated in this research. The key individual findings were:

- The production and EoL impacts of current lithium-ion batteries contribute around 10% of a BEVs lifetime CO_{2e} emissions, based on average EU scenarios. Several parameters can influence this figure, such as lifetime, the lithium-ion cell type and the in-use electricity emissions. However the battery did not drop below 5% of a BEVs total lifetime CO_{2e} emissions, unless extremely adverse conditions were assumed. Conversely, if the battery pack were to require replacement or low emission electricity was use to charge a BEV, the significance could increase to over 20%.
- Many battery production/EoL factors only have a small impact relative to that of the total vehicle's lifetime, but in absolute terms they can still represent notable changes in CO_{2e} emissions. Some of these are quantified in Table 7.4, such as the use of natural rather than artificial graphite in the anode. This alteration reduced the vehicle lifetime CO_{2e} emissions by less than one per cent, but still represented an absolute saving of over 160kg of CO_{2e}, which will cumulate dramatically at the fleet level. Seemingly small changes, even in the battery LCA, can thus still be important considerations and when combined with other minor factors form notable improvements in an overall vehicle.
- BEVs can offer whole life CO_{2e} emissions benefits, with reductions of up to 21% found against an efficient comparable diesel vehicle, using the baseline assumptions over the NEDC. However it is important to appreciate the variability surrounding the precise values, and that different metrics or scenarios could produce alternative results (see Section 7.1).
- The relative contributions of the total vehicle production and EoL phases changed significantly between the powertrains. They only represented about 20% of the diesel vehicles lifetime CO_{2e} emissions, but nearly 40% of the BEVs.
- The BEV production/EoL CO_{2e} emissions, excluding the battery, were almost as high as a complete diesel vehicle. Therefore the battery production impacts, ≈10% of lifetime CO_{2e}, essentially represented an addition relative to a conventional

vehicle and offset a corresponding proportion of the overall benefits found for BEVs. This reduction was significant, approximately abating the benefits by one third for the baseline results. For example the highest BEV benefits, shown in Figure 7.2 relative to a diesel vehicle, increased from 21% to 29% when the battery production/EoL emissions were excluded and greater increases were found for the battery types which offered lower initial benefits.

- The CO_{2e} production emissions, of the three lithium-ion battery variants assessed, deviated by up to 16% on a mass basis. This variation indicated increasing impacts with higher specific energies. However based on the batteries assessed, this trend was reversed when they were evaluated on an energy basis, due to the increased production impacts being more than offset by higher specific energies. These benefits of superior specific energy were further increased when incorporating the additional benefits of concomitant lighter packs on the in-use phase of a BEV.
- The culmination of the mechanisms attained from higher specific energy, showed approximately a 6% reduction in lifetime CO_{2e} emissions for a BEV utilising nickel cobalt manganese (NCM) cells, compared to one using lower energy lithium iron phosphate (LFP) cells. The trade-offs this necessitates with lifetime were investigated, which showed there may only be limited scenarios when the high lifetimes of LFP cells are beneficial to BEV CO_{2e} emissions. This indicated the importance of the assumed lithium-ion cells in assessments of BEVs.
- The CO_{2e} emission results exhibited by the most detailed existing lithium-ion battery LCAs available to the author (see Figure 6.10) varied greatly and appeared to suggest dramatically higher impacts for packs using NCM and LFP cells; typically more than three times those using LMO cells. The author's assessment revealed that, although there are some differences, the majority of this trend resulted from discrepancies in the assumptions and data between assessments, not from the different cell types.
- The sensitivity analysis, performed using the author's battery LCA model, suggested the deviations in production CO_{2e} emissions are likely to be far lower than the (up to) five-fold variation found in the existing literature (see Section 3.4). For example, if the impacts for any of the main battery or cell components/processes (see Figures 6.1 and 6.3) were doubled, the maximum deviation introduced would only be around one third. Larger deviations would necessitate major alterations such as, prototype production which uses very

unrefined processes, or manufacturing using materials/energy predominantly sourced from areas which employ techniques with substantially higher emissions.

- Battery recycling can be beneficial. End-of-life impacts are often excluded or only partly assessed in battery LCAs, but EoL treatment of vehicles and batteries is mandatory in the EU and should therefore be incorporated. When including the necessary processes to dismantle, separate and recover the materials, CO_{2e} reductions of up to 11% were found in the battery production values; the majority of which emanated from the non-cell components. This is far lower than the gains often reported for recovering some individual battery materials. However, to quantify the benefits of recycling, the entire pack and all processing steps need to be included, e.g. the impacts of stripping the pack and separating the cells prior to material reclamation, not just the benefits of reclaiming certain materials. Under the modelled hydrometallurgical process, only the NCM cells themselves showed benefits due to the valuable metals they contain. Process refinements are likely to improve the benefits, but recovery of materials, such as the cathode active powder for reuse in batteries without significant reprocessing, is necessary to attain substantially higher gains.
- The processes involved in removing and stripping battery packs could also pose significant economic implications for recycling, considering that EoL treatment facilities only spend an average of around 15 to 20 minutes preparing a whole vehicle prior to crushing (Brantwood Auto Recycling Ltd, 2007). For example, the hundreds or even thousands of cells, plus additional components, in an electric vehicle battery pack may need to be segregated which could take considerable time.
- Significant energy losses of around 20% are associated with current BEV charger and battery systems. These systems therefore represent an area where substantial gains could be attained, e.g. over a 3% reduction in lifetime CO_{2e} emissions were found when this loss was reduced by a quarter.
- The effects of aging and increased power demands, e.g. auxiliary draws or harsh driving cycles, clearly affect battery efficiency. The model indicated that up to 3%, of the approximate 35% in-use energy increase found for more demanding driving cycles compared to the NEDC, resulted from enhanced battery losses. The same effects were shown for the higher power rates associated with fast charging. These factors effectively lead to the sensitivity of a BEV to in-use conditions being increased and thus exaggerations in the discrepancies found between test cycles and real-world usage.
8.2.2. The need for improved assessments

The large variations in existing battery LCAs, and trends amongst different lithium-ion cathode materials, were found to result from the assumptions used and significant sharing of data. Two key contributors were the battery assembly energy and binder impacts, both of which were on their own found to account for more CO_{2e} emissions in some assessments than reported for the entire battery in others. The variation in assembly energy emanated from a lack of primary data on lithium-ion battery assembly, and the various subsequent assumptions used to fill this void. The high binder significance resulted from the use of a single dataset by several assessments that had exceptionally high CO_{2e} impacts. However, an alternative dataset for the same material found dramatically smaller impacts and, even if the high values are correct, alternative binders are available.

A lack of data on specialist battery materials, such as various cathode powders and battery separators, was found to introduce variations into results. Investigation of commonly employed datasets showed proxies/assumptions are being utilised which are substantially different to the processes used to produce some lithium-ion battery materials. Further variation was found due to multiple production routes for many battery materials and components, which utilise vastly different processes and precursors. A case study, based around battery grade graphite used in the anode, showed the assumed source of this one constituent could alter the battery CO_{2e} emissions by over 6% and those of the whole lifetime of a BEV by approaching 1%.

At the whole vehicle level battery lifetime, efficiency and mass were shown to have appreciable impacts on the findings. Battery specific energy was shown to be an important variable, but quantification of both the production and in-use benefits it brings for equal range are needed to fully appreciate its effects on BEVs. Therefore, when comparing different batteries for BEVs it is not sufficient to set a pack energy. A range should be specified to maintain utility amongst the vehicles and help ensure the true effects of a battery choice are identified.

The research focused on lithium-ion batteries for BEVs, which were found to have a significant influence on whole vehicle findings. However many of the problems discussed, concerning limited and variable data, will affect assessments of other alternative vehicles and components, such as motors, fuel cells and hydrogen vessels.

8.3. Outline framework

The framework outlined in Figure 8.1 was derived, based on the research findings contained in this thesis, to provide enhanced sustainability assessments of alternative powertrains focusing on BEVs. This helped fulfil the final project objective (Section 1.4.5). Figure 8.1 depicts the lifetime assessment in two main blocks, the vehicle production/EoL treatment and the in-use phase. Key considerations for each are then shown to feed to and from them. An important consideration is that the two main phases iterate extensively with each other rather than a simple flow from production, followed by use, and finally EoL. These interactions are necessary to allow for the important effects of choices between phases and analysis of trade-offs.

A further vital aspect of the framework surrounds the input data to the LCA models. Significant deficits were found in common input data for specialist materials used in alternative powertrains, along with variations due to assumptions, some of which are propagating through assessments. The considerations shown for the LCA input data represent some of the factors that should be checked. These aim at encouraging verification of datasets, even if commonly used in similar assessments, to ensure they provide reasonable approximations of the particular process or material that they are to represent, noting different grades (e.g. battery grade materials which may be highly pure or require specific particle sizes).

The loop for the in-use energy source shows that vehicles should not be evaluated in isolation. Resource usage, incurred by the use of a particular powertrain option, should be ensured not to preclude the use in other systems that could offer greater overall benefits, as discussed for low emissions electricity in Section 7.4.5.



Figure 8.1 Outline framework for evaluating the sustainability of advanced powertrains

The functional unit, and the comparison vehicle chosen, form another aspect of the framework. Many aspects, such as lifetime distance travelled and vehicle size compared, are typically included in the goals and scopes of assessments, as recommended by ISO 14040 (see Section 3.2.1). However, the research identified several factors that should be included in the framework, but are often overlooked in assessments. These include:

- The adoption of equivalent parameters (e.g. coefficients of drag and frontal areas) when assessing different powertrain options, i.e. not just taking vehicles with similar sizes (see Section 2.2.3), to ensure the findings are not partly due to other factors.
- The age and technology level of the comparison vehicles. There is currently a considerable pace of technological improvement in vehicles, which is creating models with significantly higher efficiencies than their predecessors. Comparing alternative powertrains that may not be realised for several years with current conventional vehicles could therefore lead to unrepresentative findings.
- The use of a set vehicle range, rather than battery mass or energy, when assessing different electric vehicle batteries. This should help ensure comparable levels of utility and that the overall effects of a battery choice are quantified.

The findings of the framework should not just report on how one vehicle compares to another, but also what the absolute savings or indeed detriments are. This should enable appreciation of the effects of alterations, such as those related to batteries given in Table 7.4, which may be relatively small compared to a vehicle's lifetime, but could nonetheless offer benefits particularly at the fleet level.

The framework is not exhaustive and has focused on the additional considerations needed for assessments of BEVs. It should be expanded as necessary to include factors specific to other powertrains and incorporate further considerations such as cost and resource requirements.

8.4. Achievements and novel contribution

The research findings and the models developed have enabled enhanced sustainability assessments of BEVs. These should help maximise benefits and ensure the desired goals of a powertrain choice are realised over the total vehicle lifetime. To achieve these benefits, improved lifecycle models were constructed and existing research was expanded upon by encompassing many factors/scenarios that have only been addressed in isolation in BEV assessments. The main contributions of the research and how they facilitated the objectives set out in Section 1.4.5, are given below:

- The construction of a new LCA for lithium-ion traction batteries and sensitivity analysis of key variables (Chapters 4 and 6). These resolved some of the issues and variability in the existing literature and permitted comparisons of several different lithium-ion options under consistent assumptions, thereby enabling more rational battery selections. The model and findings covered objectives 1 and 2 of the research (Section 1.4.5).
- The incorporation of end-of-life processing for the entire battery pack into the LCA and evaluation of the influences, beginning with removal from the vehicle. This was addressed in Sections 4.5 and 6.5 and covered objective 3.
- An evaluation of different lithium-ion batteries on the lifetime of BEVs. The overall model constructed incorporated many additional factors, which enabled some of the secondary effects and lifetime repercussions of battery choices to be evaluated. For example the in-use model constructed was developed of allow the effects of battery efficiency, typically only evaluated at the cell level in previous research, to be studied at the vehicle level. The main factors considered were:
 - The production and EoL impacts of lithium-ion batteries, together with the effects of variations in these factors, on the whole vehicle.
 - The effects of mass variations arising from different lithium-ion chemistries on in-use vehicle energy consumptions, including the secondary effects these will have on the required pack energy, and therefore production impacts, for equal utility (i.e. range).
 - The impacts of battery lifetime.
 - The effects of battery ageing.
 - Battery efficiency.
 - The results of variations in the electricity grid emissions used to charge BEVs.

These factors have been assessed to various extents in previous works. However this research has brought them together in the context of BEVs to enable trade-offs between them to be evaluated. This research covered objectives 4 (Chapter 5), 5 and 6 (Chapter 7).

• The proposal of a framework which enables enhanced quantification of the repercussions of alternative powertrain components (Section 8.3). Together with comparisons against an efficient ICE vehicle (Chapter 7) this covered the final objective (7) of the research.

The research findings (Section 8.2) showed that the inclusion and evaluation of the factors given above can have important repercussions on the results. This means that more holistic frameworks are needed, which identify and incorporate the additional important variables and trade-offs involved in powertrain assessments, thereby validating the research hypothesis given in Section 1.4.3.

The research described in this thesis is further supplemented by several published contributions (see Appendix A). For example Sweeting, et al. (2011) studied the effects accessory power draws can have on BEV energy consumption which, considering the scale of the possible impacts found, had received little attention in the existing literature.

8.5. Suggestions for future research

The research revealed many variables in vehicle lifecycles and areas surrounding the input data for LCAs of alternative powertrains that require improved quantification. The list below summarises the most critical areas identified that would enable more comprehensive LCAs of alternative powertrains. Further research is needed to:

- Verify and improve LCA inventory data for key battery materials and processes. Some improvements can be attained by ensuring data is representative and reasonable. However, primary data is needed from manufacturers for the large scale production of electric vehicle batteries and materials, to provide verification of factors such as the requirements of battery assembly.
- Incorporate the effects of other impacts. This assessment evaluated CO_{2e} emissions, but there are many other important emissions and factors, such as cost and resource depletion, that need to be accounted for when assessing alternative vehicles. Substantial further work is needed though in the background data to ensure the validity of results for many of these factors.

- Assess the potential of other batteries and the trade-offs these may introduce. This should entail further lithium-ion variants and other battery types, such as zinc and lithium air batteries, that may be suitable for future electric vehicles.
- Better quantify the lifetimes of batteries under real-world usage in BEVs and evaluate lifetime trade-offs.
- Provide improved quantification of the losses associated with electric vehicle battery and charger systems. This should cover further investigation of variations due to for example ageing, temperature and charging rate on vehicle performances, as well as work to help mitigate this currently substantial area of loss.

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