Economic and Environmental Impact Analysis of MWCNT Lithium Nickel Manganese Cobalt Oxide Batteries Manufacturing Considering Worker Safety

A Dissertation Presented

By

ALI HAKIMIAN

To

The Department of Mechanical and Industrial Engineering

in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

in the field of

Industrial Engineering

Northeastern University

Boston, Massachusetts

April 2015

ABSTRACT

Development of safe, economically competitive, and environmentally responsible nano-enabled products, is a desired outcome to avoid unintended consequences for the use of nanomaterials. Carbon nanotubes (CNTs) offer great potential for improving the conductivity and capacity of lithium-ion batteries, but concern for potential impacts on human health and the environment could delay implementation. Given the uncertain risks, additional precautions for exposure prevention may be warranted, although not yet regulated. Companies working with engineered nanomaterials (ENMs) may need to explore decision tradeoffs for additional occupational safety costs and the environmental impacts.

Currently under research, multi-walled carbon nanotube lithium nickel manganese cobalt oxide batteries (MWCNT NMC batteries) show greater energy density and product life than existing lithium-ion batteries. To explore the economics for manufacturing scale-up, a stochastic process based cost model was developed to investigate the cost drivers for manufacture of MWCNT NMC batteries, targeted for satellite and computer applications. In the model, various occupational safety scenarios were considered to analyze the effect of different levels of prevention for worker exposure on the total manufacturing cost. Multi-criteria decision analysis (MCDA) methodology was applied to prioritize a range of alternatives for decision makers, using AHP techniques to recommend best alternatives for each stakeholder. A benefit-cost ratio analysis was also performed to categorize the most desirable product for the decision makers.

To assess the environmental impacts of the manufacturing of CNT lithium-ion batteries, a life cycle assessment (LCA) methodology was applied. Inventories were generated using scenarios from the cost model and used to evaluate the environmental impacts in the manufacturing stage with SimaPro™ software. Results provided 1) a first order environmental footprint on the manufacturing process for scale-up, and 2) insights on potential process improvements given the uncertainty in regulatory constraints for nanomaterials. Further, by adjusting the input assumptions, sustainable manufacturing practices for MWCNT NMC batteries with renewable energy (solar energy) use were explored.

Using various methodologies, concurrent assessment of the economic and the environmental health and safety tradeoffs for manufacturing scale-up was explored for MWCNT lithium-ion batteries to determine the economic feasibility, given the uncertain exposure effects of CNTs. The results not only allow consideration of strategies to reduce the manufacturing costs and to utilize sustainable manufacturing practices, but also help manufacturers to estimate the economic viability associated with alternative processing methods to avoid worker exposures. Results from this work offer economic, environmental, health and safety tradeoff analyses to promote sustainable nanomanufacturing.

Acknowledgements

First and foremost, I would like to thank my dissertation advisor, Prof. Jacqueline Isaacs for her guidance, patience, and support over the last five years. I would also like to thank my committee members, Prof. Sagar Kamarthi, Prof. Thomas Cullinane, and Prof. K.M. Abraham for their guidance throughout my PhD program.

I would also like to thank Prof. Christopher Bosso and all the members of SNM group. It was my great pleasure to work with you all.

I would like to extend my sincere thanks to Prof. Ahmed Busnaina, Dr. Sivasubramanian Somu, staff, and all the graduate students at CHN in Northeastern University.

My deepest gratitude goes to my colleague Serkan Erbis for being such an incredible person, teammate, and friend.

Most importantly, I would like to acknowledge my greatest appreciation to my parents, Batool and Abbas Hakimian, my sister, Hoda, my nieces, Hasti and Delara for their endless love and support in my life. Last of all, thank you to my wife, Sofia for being the love of my life and being so supportive. Words cannot describe how grateful I am for your support.

Table of Contents

List of Figures

List of Tables

CHAPTER 1 INTRODUCTION

Improvements in synthesizing nanoscale materials and controlling their properties have contributed to their use in broad areas of application including advanced materials, electronics, magnetic and optoelectronics, biomedicine, pharmaceuticals, cosmetics, energy, catalytic and environmental detection and monitoring, and energy storage devices (Agency 2007, Wen-Tso 2007) . The nanoscale dimensions (with at least one dimension less than 100 nm) in nanomaterials contribute to their unique physical, chemical, and biological characteristics. The distinctive properties of nanomaterials offer the promise of great advances in many scientific and technological areas (Agency 2007). The impact of nano-enabled products across the global economy has been estimated to grow at a minimum to $3.3 trillion in 2018 (Research 2012). In the United States, the cumulative investment increased technology development is estimated to be $ 21 billion since the inception of the National Technology Initiative (NNI) from 2001 through 2016 (Council 2014).

Despite of all of the positive aspects and functional performance of nanotechnology, researchers anticipate that there may be potential negative implications of using nanotechnology on the environment, human health, and safety in addition of being costly (Aasgeir Helland 2007, Maes, Schaeffer et al. 2009, Stander and Theodore 2011). Because nanotechnology is an emerging technology, questions remain regarding environmental safety and human health; the potential for harm after exposure to nanomaterials has not been fully characterized. Potential exposure to nanomaterials can be including oral, dermal, injection, and inhalation. Therefore, assessing the nanotechnology benefits and risks to understand their potential environmental and human health impacts has been one of the key research topics. The cumulative investment in the environmental, health, and safety (EHS) research area – through more limited than the overall investment for research and development- has reached almost $1billion between 2006 and 2016 in the United States (Council 2014).

1.1. Carbon Nanotubes Structure and Properties

The use of carbon nanotubes (CNTs) in different products is of high interest in many industries, because of their remarkable properties. CNTs are nano-scale allotropes of carbon that have a cylindrical structure (Dresselhaus, Dresselhaus et al. 2004) . The diameter of a CNT is normally only a few nanometers, however, its length can be up to a few millimeters. Their structure, as well as their exclusive electrical, mechanical, thermal and magnetic properties place them in a special class of materials for many potential industrial and scientific applications (Dresselhaus, Dresselhaus et al. 2004, Han, Yick et al. 2011). In addition, their unique chemical properties can lead to phenomenal efficiency enhancement, improved durability, conductivity, and mechanical strength of products (Lee, Mahendra et al. 2010, Initiative 2013). Produced as single-walled carbon nanotubes (SWCNTs) or multi-walled carbon nanotubes (MWCNTs), they are light-weight high-strength materials (Baughman 2002, Han, Yick et al. 2011). SWCNTs consist of a single graphene sheet with a cylindrical shape, whereas MWCNTs consist of two or more of these cylindrical graphene sheets of different diameters that are stacked inside each other (Leonard 2007). They are assumed in three different chiralities: armchair, zigzag, and chiral. These chiralities are defined by the chiral vector (Peng, Yan et al. 2003, Leonard 2007). Depending on their chiralities, CNTs conductivity is varied, resulting in either metallic or semiconducting properties (Han, Yick et al. 2011, Caitlin Fisher 2012) .

There are four different methods for manufacturing CNTs including: arc discharge (arc), laser ablation, chemical vapor deposition (CVD), and high-pressure carbon monoxide (HiPco) (Dresselhaus 2008, Meagan L. Healy 2008). Arc discharge and laser ablation are techniques that use graphite as a feedstock in order to synthesize CNTs, whereas the CVD method uses a variety of hydrocarbon feedstocks, where solid and liquid hydrocarbon can be employed (Dunens, MacKenzie et al. 2010). In the HiPco method, CO is being used as the carbon precursor for producing CNTs (Meagan L. Healy 2008, Venkata Upadhyayula 2011) .

1.1.1. Environmental and Human Health Issues

The growing use of nanomaterials has consequently resulted in increasing concerns for their potential negative impact on human health and the environment. There is significant uncertainty regarding the environmental and human health impacts of CNTs due to limited data on their long term environmental effects. Some of the lab studies report that CNTs are more toxic than carbon black in mice lungs and may cause some inflammation and fibrosis (Shvedova 2008, Teow, Asharani et al. 2011, Hsieh, Bello et al. 2012, Sharifi, Behzadi et al. 2012) . It is also apparent that CNTs and nanoparticle reactivity and toxicity might depend on their size, surface chemistry, surface area, shape, aggregation and other physiochemical factors (El-Ansary and Al-Daihan 2009).

Depending on the application, release of CNTs could occur during the CNT production process, manufacture of nano-enabled products, use-phase, and/or product recycling / disposal phase (Aasgeir Helland 2007, Maes, Schaeffer et al. 2009, Olapiriyakul 2010, Stander 2011). CNT releases during manufacture can be categorized as direct or indirect. Direct releases into air could occur during transportation or through spills, while indirect releases can happen when treated or untreated wastewater somehow reaches a river or landfill (Fadri Gottschalk 2010, Olapiriyakul 2010).

Therefore, as a precaution, and with the uncertainties for nanomaterials possible toxicity effects, it is essential to consider additional safety parameters to avoid exposure to and releases of nano-elements throughout the life cycle of nano-enabled products (NEPs) (Agency 2011, NIOSH 2013) .

1.1.2. Market and Applications

The market demand for CNTs is expected to increase considerably in the future (Nanowerk 2011, Kozarsky 2014) . The global market demand for CNTs is anticipated to rise 40 to 50% in 2016 relative to what was in 2011 (Nanowerk 2011). Studies show that the market demand for MWCNTs will reach 3728 MT by 2020 compared with 200 MT in 2011 (Kozarsky 2014). In 2014, Lux Research reported that the future demand of MWCNTs will result from two applications, namely, conductive polymer composites and lithium-ion battery electrodes (Kozarsky 2014) . Figure 1-1 shows the MWCNT global market demand for conductive polymer composites and lithium-ion battery electrodes.

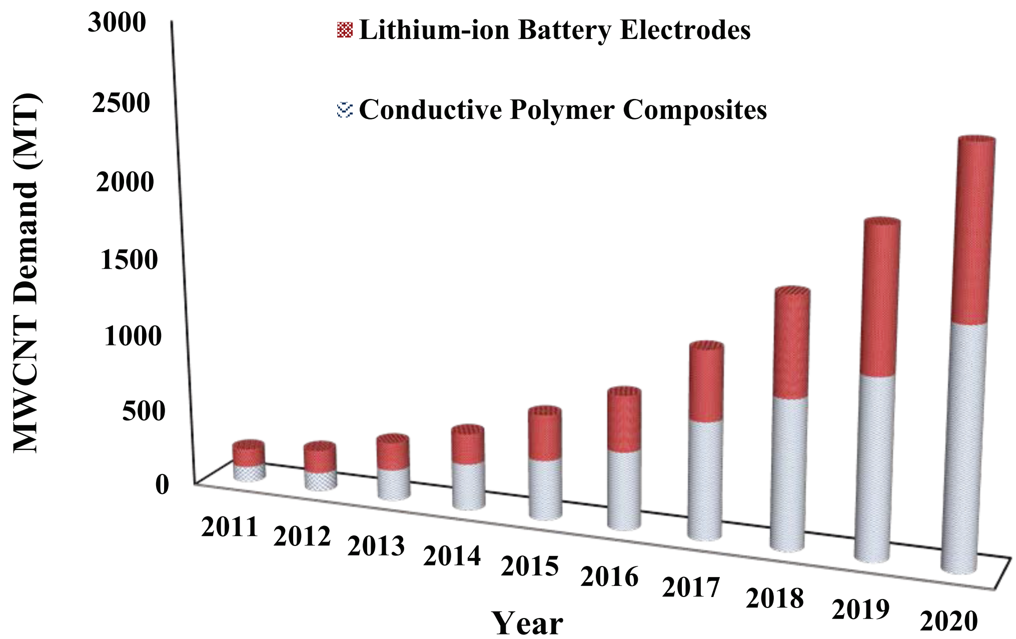


Figure 1-1 Anticipated MWCNT global market demand (Kozarsky 2014)

1.2. MWCNT Lithium-Ion Battery Overview

In this study, the device under investigation is MWCNT lithium nickel manganese cobalt oxide (NMC) batteries which are at the research and development stage (Shah, Ates et al. 2014). CNTs have great potential for improving the lithium-ion battery performance when included as an additive in lithium-ion batteries. They can be either added to the cathode cell to enhance its performance or to be used as a replacement for graphite in the anode cells (Jin, Gu et al. 2008, Zhang, Cao et al. 2010). CNT in the cathode cells puts them in constant contact with both the electrolyte and the aluminum current collector. The high chemical resistance of CNTs against the reactivity of lithium-ion cells and other solvents make CNTs an ideal additive material to cathode cells. Other benefits of adding CNTs in the batteries include: improved electronic conductivity of the cathode electrode, increased charge/discharge rate capability, and higher structure flexibility (Jin, Gu et al. 2008, Zhang, Cao et al. 2010) . While the remarkable electrical, thermal, and mechanical properties of CNTs are important in other applications, their addition in lithium-ion batteries is expected to result in safer and longer product cycle life (Che, Cagin et al. 2000, Lasjaunias 2003, Landi, Ganter et al. 2009). With high voltages and electric current in the battery cell, low flammability materials such as CNTs are desired.

1.3. Research Objectives

In recent years, sustainable manufacturing and conservation of natural resources have become major challenges of global economics (Programme 2011). As a part of the nanomanufacturing and sustainability research at Northeastern University, the overall aim of this work is to develop a comprehensive economic impact analysis of the scale-up for manufacturing of the next generation of lithium-ion batteries, while assessing the environmental impacts of materials, resources, and equipment. Further, by adjusting the input assumptions, sustainable strategies during manufacturing processes are investigated. These methods are applied for CNT lithium-ion batteries with targeted application of satellites and portable computers. Different levels of occupational safety protection during production are explored. Figure 1-2 describes various life cycle phases of products and emphasizes of assessing the economic and environmental manufacturing phase of batteries in this study.

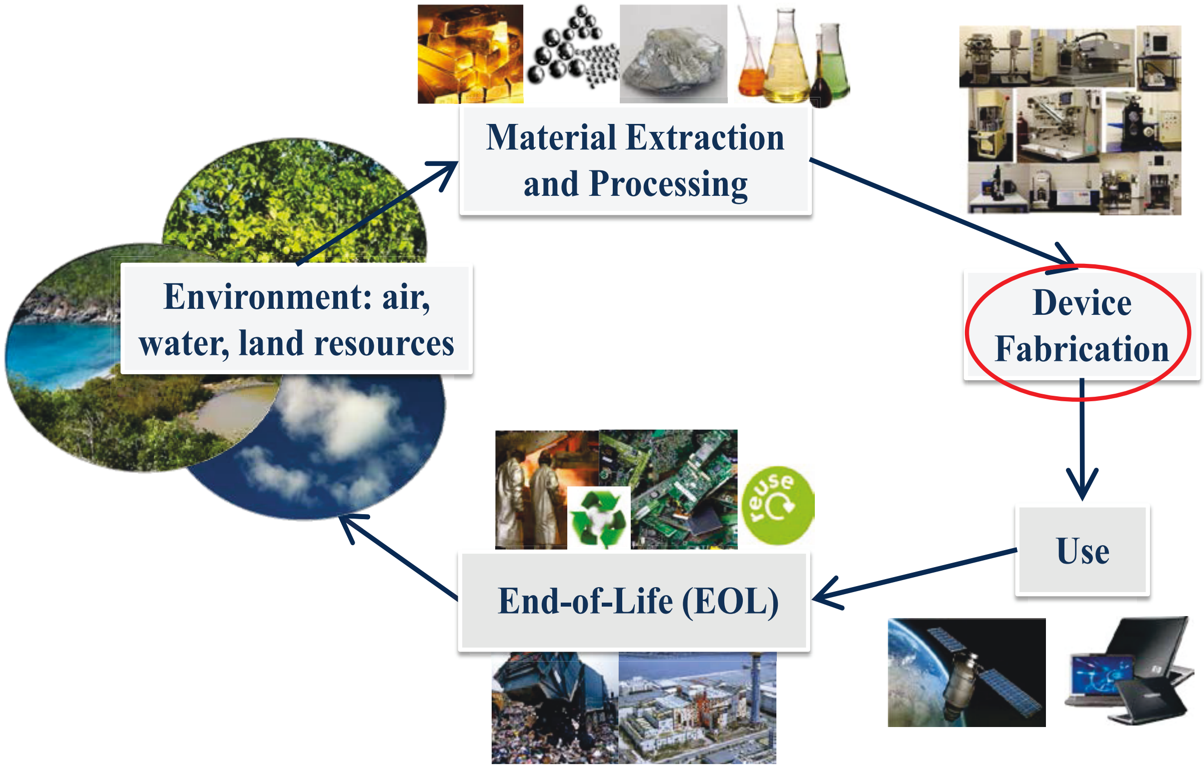


Figure 1-2 Economic and environmental analysis of manufacturing phase in the life cycle of CNT lithium-ion batteries for satellites and portable computers

The specific aims of this work are:

1- To develop a stochastic process-based cost model (PBCM) that accounts for uncertain cost parameters and calculate the average cost and the cost intervals of the MWCNT NMC batteries by using the Monte Carlo simulation technique and generating results for each uncertain parameter

1a: To explore alternative environmental health and safety practices during the MWCNT NMC batteries manufacturing and investigate the decision tradeoffs for additional occupational safety costs.

1b: To explore sustainable manufacturing practices for MWCNT NMC batteries with renewable energy (solar energy) use; and the resulting environmental impacts.

2- To investigate the environmental implications of manufacturing phase of MWCNT NMC batteries by applying life cycle assessment (LCA) methodology, and to explore decision tradeoffs for the cost of sustainable energy technology adoption and the environmental impacts.

3- To identify the most desirable alternative (from various decision makers' perspectives) among different options (various types of produced batteries) and develop multi criteria decision analysis (MCDA) by applying analytical hierarchy process (AHP) methodology.

1.4. Executive Summary

Following the scope and executive summary provided in Chapter 1, Chapter 2 provides a thorough literature review on the state-of the-art in lithium ion batteries. Different types of lithium-ion batteries, cell designs, the working principle of lithium-ion batteries, and the targeted applications (satellites and portable computers) are also discussed in Chapter 2. In Chapter 3, the economic analysis of MWCNT NMC batteries is developed by applying a process-based cost modeling approach. Different levels of occupational safety standards (low, medium, and high) during the battery production are established. Chapter 4 evaluates the environmental impact assessment of MWCNT NMC batteries by applying the life cycle assessment methodology, and explores use of the sustainable energy technology. In Chapter 5, multi criteria decision analysis methodology is used to select the best choice (from decision makers' perspectives) among different alternatives (various types of produced batteries). Finally Chapter 6 provides conclusions of the work and outlines future directions.

CHAPTER 2 STATE-OF-ART: BATTERY

2.1. Battery System

A battery is a portable energy source which consists of three solid components: anode, cathode, and separator which are installed in a liquid or electrolyte solution. The anode is the negative part of a battery (Battery Handbook). The cathode is the positive section of a battery and the electrolyte is a conductive solution which contains acid or alkaline electrolytes in conventional aqueous batteries or lithium salt solutions in organic solvents in lithium batteries (ChemPages 2012, Buchman 2013). On discharge, electrons and ions flow from the anode to cathode, ions inside the battery cell and the electrons through the external load circuit. While the battery is being charged, electrons travel in the reverse direction (Goodenough 2012). Figure 2-1 shows the schematic of a typical battery.

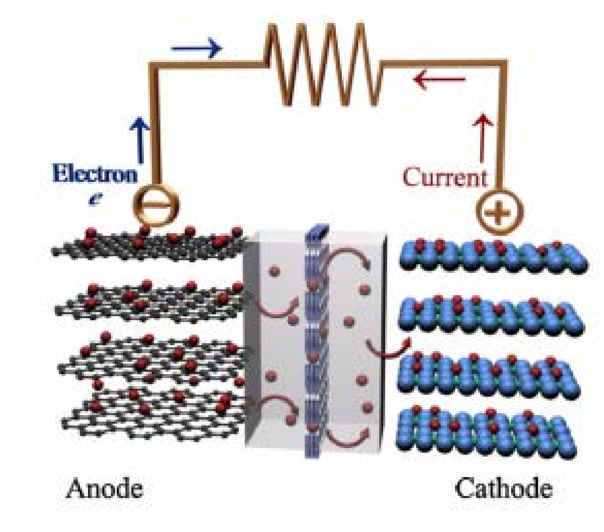


Figure 2-1 Schematic of a typical battery (Song, Park et al. 2011)

Two main classifications for batteries are primary or non-rechargeable and secondary or rechargeable. Primary batteries have high specific energy and long storage times. These types of batteries can be used when charging is impossible or not practical (Song, Park et al. 2011, Goodenough 2012, Kubis 2012) . They are usually environmentally friendly. Some applications of primary batteries are wristwatches, remote controls, electric keys, children's toys, and pacemakers for heart patients (Buchman 2013). The most common use for secondary or rechargeable batteries is for electric vehicles, telecommunications, emergency and backup power, and portable electronic devices (Kularatna 2011). Batteries could be in different shapes and sizes. They are distinguished and classified by their properties such as, chemistry, voltage, capacity, and power (Buchman 2013). Some batteries have high capacity but they would not deliver much power. On the other hand, there are some batteries with low capacity with a capability of delivering a lot of power like the batteries which are used to start up engines. A battery can function as a single cell to power a cellphone or operate as multiple cells to power a vehicle (Kubis 2012, Buchman 2013).

The most common rechargeable batteries are nickel, lead, and lithium-based systems with different charging algorithms and different regulatory requirements. A different charging algorithm means, different batteries with various chemistries are not interchangeable in the same charger (Kularatna 2011). Rechargeable batteries with different chemistries are discussed below.

2.2. Battery Types

2.2.1. Lead- based batteries

Lead acid batteries are the first researchable batteries which have been used for commercial purposes. The positive electrode of these types of batteries is lead dioxide while metallic lead is used as the negative active material (De Andrade, Impinnisi et al. 2011, Buchman 2013). The electrolyte solution is sulfuric acid. Lead-acid batteries have been used in various applications such as; starting, lighting, and ignition of gasoline-powered cars, electric cars and, grid energy storage (Zhang, Zhao et al. 2012). Lead-acid batteries are inexpensive and simple to manufacture. They are capable of performing well in low and high temperatures. However, there are some drawbacks and limitations of using these batteries such as; a charging period, which would be relatively long (Kubis 2012, Snyders, Ferg et al. 2012). Also, in order to prevent them from sulfation, they must be stored in the charged condition. They have a limited life cycle. Charging lead-acid batteries repeatedly reduces the battery-life significantly. Finally, they are not environmentally friendly (Gottesfeld and Pokhrel 2011).

2.2.2. Nickel-based batteries

The first generation of nickel-based batteries was nickel-cadmium (Ni-Cd) batteries which were invented in 1899 and offered numerous advantages compared with lead-acid batteries (Buchman 2013). In these types of batteries the positive electrode was nickel hydroxide while the negative electrode was cadmium (Gaines 2010, Kubis 2012). Nickel-based batteries were used when extended temperature range and high discharge rate was essential. Nickel- cadmium batteries were charged fast, even if they had been stored for a considerable period of time. The number of charge/discharge cycles of nickel-cadmium batteries was high and had a good-low temperature performance (Gaines 2010). On the other hand, there were some boundaries in regards of using Ni-Cd batteries, such as; having relatively low energy density or being environmentally unfriendly because of the cadmium which is a toxic metal (Huang, Li et al. 2010).

These limitations made scientists start developing the new generation of nickel-based batteries. Nickel-metal-hydride (NiMH) batteries had the 30-40 percent higher capacity compared with standard Ni-Cd batteries and were environmentally friendly (Gaines 2010). These types of batteries are mainly used in hybrid electric vehicles and for starting aircraft. They even have some advantages over the newer battery technology- lithium-ion batteries- in terms of safety and price which will be discussed later. Using NiMH batteries having some limitations, for instance; they have limited service life and require complex charging algorithms (Gaines 2010, Buchman 2013).

2.2.3. Lithium-based batteries

Lithium based batteries are the fastest growing battery system. Lithium's properties make it the ideal metal for a battery (University 2012). It is lightweight and provides the largest specific energy and power density per weight (Cheng, Liang et al. 2011). Developing lithium-ion batteries, first, started in 1970. Commercially production happened in 1991 (Armand and Tarascon 2008, Sankey, Clark et al. 2010). Lithium metal features the lowest anode potential, which causes the highest potential difference between the anode and the cathode, and thus the cell voltage, is maximized (University 2012). Having high cell voltage and superior energy density makes lithium-ion batteries to be replaced other batteries in different type of applications (Armand and Tarascon 2008).

Compared with lead acid or nickel-metal-hydride cells, lithium-ion cells provide a cell structure that operates two times longer (Antti and Justin 2012). Moreover, in batteries which contain lithium, the self-discharge is less than half compared to nickel-cadmium batteries (Buchman 2013). However, using lithium-ion in batteries has some drawbacks. Manufacturing lithium-ion batteries is costly. Lithium-ions require a protection circuit to sustain a safe operation. Also, lithium is a reactive metal and has a low cycle life particularly under high current densities (Antti and Justin 2012). In addition, lithium-ion cells are sensitive to high and low temperature (Chong, Xun et al. 2011).

2.2.4. Characterization of different types of secondary batteries

Advancement in batteries is evaluated based on the batteries characterizations and specifications, such as; their specific power and energy. Specific energy is the capacity a battery can hold and specific power is the battery's capability to provide power (Antti and Justin 2012). Table 2-1 summarizes the energy and other characterizations of lead acid, nickel-cadmium, nickel-metal-hydride, and the lithium-ion batteries family.

Table 2-1 Specifications of secondary batteries

Specifications	Lead Acid	NiCd	NiMH	Li-ion		
				Cobalt	Manganese	Phosphate
Specific energy (Wh/Kg)	30-50	45-80	60-120	150-190	100-135	90-120
Life cycle	200-300	1000	300-500	500-1000	500-1000	1000-2000
Fast-charge time	8-16h	1h	2-4hr	2-4h	1h or less	1h or less
Self-discharge/month (room temp)	5%	20%	30%	<10%		
Charge temp	(-4 to122°F)	(32 to 113°F)		(32 to 113°F)		
Peak load current	0.2C - 5C	1C-20C	0.5C-5C	<1C & >3C	<10C & >30C	<10C & >30C
Cell voltage	2V	1.2V	1.2V	3.6V	3.8V	3.3V
Discharge temp	(-4 to 122°F)	(-4 to 140°F)		(-4 to 140°F)		
Maintenance requirement	3 - 6 months	30-60 days	60-90 days	Not required		
Safety requirement	Thermally stable	Thermally stable		Protection circuit mandatory		
Toxicity	Very high	Very high	Low	Low		

As shown in Table 2-1, the lithium-ion batteries family is better compared with other rechargeable batteries in terms of energy and power density. Because of these advantages, researchers say the lithium-ion batteries will dominate the electric automotive transportation, portable electronic devices, and renewable energy storage markets in a near future (Kathy Hart 2012).

2.3. Lithium-Ion Battery Technology

A conventional lithium-ion battery cell, as shown in Figure 2.1, is built up of three solid components including cathode, separator and anode, which are immersed in a liquid electrolytic solution (Thackeray, Wolverton et al. 2012). The shape of lithium-ion batteries varies and depends on the targeted applications. Some of the more common shape of batteries is cylindrical, prismatic, and pouch cells (C. Mikolajczak 2011). To protect a lithium-ion battery against false charging or critical temperature, having a battery management system (BMS) as one of the battery components is essential (Buchman 2013). In commercial lithium-ion batteries, the cathodes (negative electrodes) and anodes (positive electrodes) are made of metallic current collectors which are coated with different types of metal oxides on the cathodes and graphitic carbons on the anodes (B. Ketterer 2009, Scrosati and Garche 2010).

In most cases, the cathodes' current collector sheets in lithium-ion batteries are made of aluminum and coated with different active materials (Armand and Tarascon 2008, B. Ketterer 2009). In a lithium-ion cell, the mass of cathode active material is larger than the mass of anode material since the energy capacity of regular graphite anodes is bigger than the capacity of cathode active materials. Thus, the cathode active material has a bigger influence on total batteries' weight since more cathode material is needed in a cell (Armand and Tarascon 2008).

In lithium-ion batteries, the choice of a cathode gives them their exclusive character. Common cathode materials in lithium-ion batteries are lithium cobalt oxide, lithium manganese oxide, lithium iron phosphate, and lithium nickel manganese cobalt (Long 2011, Antti and Justin 2012, Sullivan and Gaines 2012). Different cathode materials in lithium-ion batteries will be discussed in details in Chapter 2.3.

The anodes' current collector sheets in lithium-ion batteries are made of copper and coated with conductive additives and a binder such as Polyvinylidene Fluoride (PVDF) (Zaghib, Dontigny et al. 2011). Although, there are few choices for anodes active materials in lithium-ion batteries include lithium metal, lithium titanate, and silicon but carbon-based anodes are the most common choice in lithium-ion batteries (Landi, Ganter et al. 2009, Zaghib, Dontigny et al. 2011).

In the 1980s, lithium-ion batteries were built by having a metal oxide cathode and a lithium anode. Having the anode made of lithium resulted in a higher voltage and a higher capacity in the battery. However, it raised many safety concerns due to increasing the temperature inside the battery cell (Trahey, Johnson et al. 2011). To prevent battery overheating and having a safer product, graphitic carbon materials were chosen as a replacement for lithium anodes (Joho, Rykart et al. 2001).

For next generation of lithium-ion batteries, silicon can be a suitable alternative for graphite anodes due to its high capacity. Replacing graphite with silicon in the anode increases the storage capacity of the battery during the charging process and significantly improves the energy density of the cell as the weight of the anode reduces (Chan, Peng et al. 2008, Landi, Ganter et al. 2009, Wu, Chan et al. 2012). However, this extreme growth in the storage capacity causes the cracks in the silicon and therefore, fast anode degradation (Zang and Zhao 2012).

The battery electrodes (anodes and cathodes) are separated by a porous polymer which is usually composed of polyethylene or polypropylene (B. Ketterer 2009). A separator helps to prevent an electrical short between the cathodes and anodes. In some cases, ceramic particles are coated to the plastic membranes and exhibited as a high temperature resistance separator (Zhang 2007). Thus battery cells' safety improves significantly.

The electrolyte provides for ion conductivity between the cathode and the anode. An electrolyte in lithium-ion batteries is a lithium salt which is dissolved in an organic solvent solution (Xu 2004, Ishikawa, Sugimoto et al. 2006, Lewandowski and Świderska-Mocek 2009). To avoid having the chemical reaction of lithium salt with water, electrolyte solvents must be water free (Ishikawa, Sugimoto et al. 2006). One of the main components of different electrolytes is their conductive salts. The most commonly used conductive salts in lithium-ion batteries which performs good ion conductivity and high oxidation resistance is lithium hexafluorophosphate (LiPF6) (Xu 2004).

As any other secondary batteries, electrochemical energy can be reversibly converted to electrical energy during charging and discharging process. As a battery operates (discharges), the lithium-ions flow from anode to cathode through electrolyte and separator (Scrosati and Garche 2010, Cheng, Liang et al. 2011, Antti and Justin 2012, Yoshino 2012). When the battery discharges, the lithium-ions are extracted from the positive electrodes (anodes), get solvated into electrolyte, and inserted into the negative electrodes (cathodes). The battery is fully discharged when all lithium-ions are intercalated in the cathode (B. Ketterer 2009). The direction of lithium-ions is reversed from the anode to the cathode when the battery is being charged. During the charging process, the lithium-ions are inserted into the positive electrodes. The charging process is completed when all the lithium-ions flow from cathode to anode and intercalated in the anode (B. Ketterer 2009). During charging process, having an external power source is essential. Figure 2-2 illustrates the charging /discharging process.

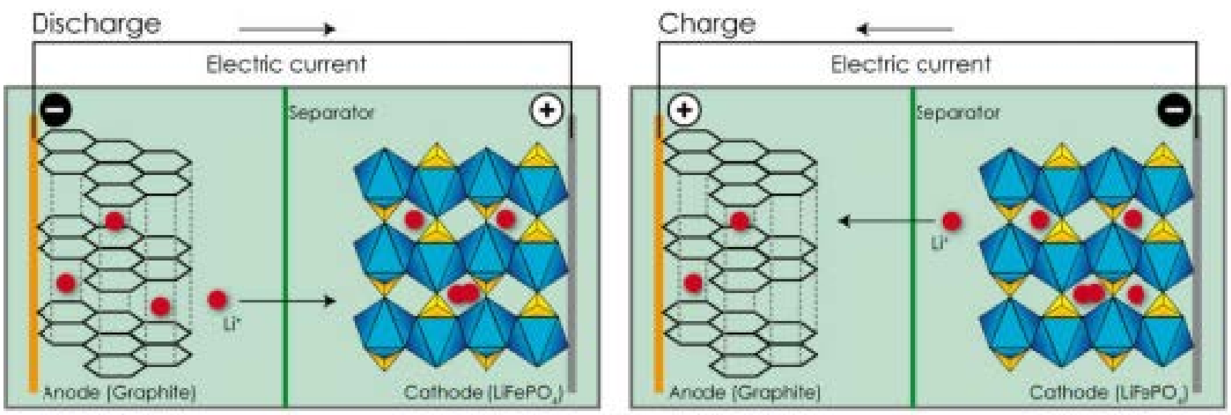


Figure 2-2 Ion flows in lithium-ion batteries during charging and discharging (B. Ketterer 2009)

During the charging and discharging process, transferring of lithium-ions between cathodes and anodes occurs with greater than 99% efficiency, therefore; the battery cells are capable to be charged/discharged over 300-500 cycles with minimum loss in storage capacity energy (Shim and Striebel 2003, Smith, Burns et al. 2010, Burns, Kassam et al. 2013). Depending on the battery cell chemistry, the battery can be charged/discharged up to ten thousand cycles if used in its respected tolerance range (Zaghib, Dontigny et al. 2011). To prevent fast degradation of a battery cell, neither cathode nor anode is completely filled/depleted with lithium-ions during charging/discharging process (Zhou, Qian et al. 2011). Moreover, to avoid short lifetime of a battery cell, lithium-ion cells should be neither overcharged nor deep discharged (Aurbach, Talyosef et al. 2004).

Lithium-ion cells are also sensitive to low and high temperatures. The range of cell batteries' working temperatures changes from -40^{C} to 80^{C} and strongly depends on the battery cell chemistry (Zhou, Qian et al. 2011). When longer lifetime is desired, a smaller temperature range between 15^{C} and 30^{C} is needed (Wang, Liu et al. 2011). The lithium-ion battery is overheated when the battery cells' temperature is raised beyond a certain point. As a result of overheating, the cathode active materials and the components of the electrolyte react exothermally (B. Ketterer 2009). If the temperature continues to rise, the separators start to melt and cause short-circuits in the battery (Long 2011). To prevent overheating lithium-ion batteries and making them safer products, various safety measures can be considered. Some safety measures include applying safer cell packaging and using temperature-resistance ceramic-enhanced separators (Antti and Justin 2012).

The average voltage and discharge capacity of the battery is directly related to the cathode chemistry. A higher voltage and capacity would provide the larger energy. Specific capacity of the cathode refers to the capacity per mass of active cathode materials without considering the mass of other cathode components such as binder and conductive additive materials. Specific energy refers to energy per unit mass while energy density the amount of energy stored per unit volume. The electrochemical capacity and energy in batteries is dependent on the constant current rate, which is often referred to as C-rate. C-rate and other important testing terms and formulas are summarized and defined below.

C-rate - C/t rates (where t is the time for a complete charge or discharge in hours) (1)

$$\textbf{Specific Capacity (mA/g)} = \frac{\text{Current (mA)*time (h)}}{\text{Active Mass (g)}} \quad (2)$$

$$\textbf{Specific Energy (Wh/kg)} = \frac{\text{Capacity (Ah) * Voltage (V)}}{\text{Total Cell Mass (kg)}} \quad (3)$$

$$\textbf{Energy density (Wh/liter)} = \frac{\text{Capacity (Ah) * Voltage (V)}}{\text{Total Cell volume}} \quad (4)$$

2.3.1. Fabrication, containment, and battery management

Lithium-ion cells are hermetically sealed and protected against oxygen, water, and other environmental influences. Battery packs are constructed by connecting the cells in series and parallel to obtain the desired voltage and current output. The cells in the battery pack are protected against overcharge and over-discharge and the capacities of the individual cells in the pack are equalized during charge by means of the electronic battery management system (Battery Handbook). The lithium-ion cell components including cathode, anode, and the separator are contained in a sealed container to prevent the battery emission components and protect the environment. As mentioned earlier, the common lithium-ion cell designs include cylindrical, pouch, and prismatic cells (Buchman 2013). Depending on the targeted applications and the desired battery shape, lithium-ion cell designs are changed. If the need of mechanical stability against both internal and external pressure is essential, cylindrical lithium-ion cells are the best option while prismatic and pouch lithium-ion cells offer a high surface area for heat transfer by having the flat shape (B. Ketterer 2009). In reality, pouch cells might become the most desired cell design due to their inexpensive construction, smaller shape and the better heat transferring ability (ChemPages 2012). To have more stability, lithium-ion cells are arranged in a case which is called battery module. The modules are installed in a battery pack. Each large battery pack could contain several modules depending on the desired power and energy density. As explained in Chapter 2.1.2. BMS is an essential battery component to improve the performance and the safety of the battery. BMS is used to utilize cell, module and battery pack surveillance (B. Ketterer 2009). In the cell level, cell management system verifies the voltage, current and temperature of each cell (Hartmann II 2008) while the module management system enables the modules to adjust the cell performances when the demand increases (B. Ketterer 2009). Therefore, it stabilizes the modules' performance. On the battery pack level, BMS constantly provides surveillance of the battery power and the remaining capacity. Also, it verifies the battery's state of charge and its overall condition (Hartmann II 2008).

2.4. Comparisons of Lithium-Ion Batteries

2.4.1. Lithium cobalt oxide

Lithium-cobalt oxide was the first active cathode material which has been wildly used in cellphones, digital cameras, and laptops because of their highly specific energy (Etacheri, Marom et al. 2011). The battery is made of cobalt oxide cathode and a graphite carbon anode. It has highly specific energy and a cell voltage of 3.6V (Zhang 2011). Despite of all cobalt advantages, using it in batteries raises big concerns. Cobalt is a very toxic material and has significant environmental impacts. Besides, it is a rare and expensive metal (Etacheri, Marom et al. 2011). Some studies show that earth's cobalt resources are limited and they will not be able to fulfill lithium-ion batteries demand by 2050 (Zimmermann 2012).

2.4.2. Lithium manganese oxide

Another type of material which is used as a cathode in the lithium-ion battery family is lithium manganese oxide. Unlike cobalt, manganese is an environmentally friendly metal (Antti and Justin 2012). Lithium manganese oxide has a high cell voltage which is 3.8-3.9V per cell. Thus, the power density which lithium manganese oxide batteries offer is high but they have a lower energy density than cobalt based batteries (Zhang 2011). The main applications of manganese based batteries are power tools, medical instruments, and electric cars due to their high power density (Scrosati and Garche 2010).

2.4.3. Lithium iron phosphate

Another alternative for the cathode materials in lithium-ion batteries is lithium iron phosphate. In comparison with cobalt and manganese, iron phosphate remains chemically stable at high temperatures even without any surrounding lithium ions (Antti and Justin 2012). Lithium iron phosphate has a high current rating and long cycle life (Xu, Chen et al. 2009). The disadvantage of lithium iron phosphate in comparison with other active cathode materials is having a smaller voltage which is 3.2V and therefore has a lower energy density than cobalt-based batteries (Zhang 2011). Due to their high performance and high safety, lithium iron phosphate batteries are mainly used in the automotive industry (Zackrisson, Avellán et al. 2010).

2.4.4. Lithium nickel manganese cobalt oxide

In this type of lithium ion battery, cathode is made by combining nickel, manganese, and cobalt. As it was demonstrated in previous parts, nickel has high specific energy but low stability and manganese offers lower specific energy but low internal resistance. By combining nickel and manganese, the best of each can be obtained (Buchman 2013). Lithium nickel manganese cobalt oxide has a 3.7 voltage cell (Scrosati and Garche 2010). The main application of lithium nickel manganese cobalt oxide batteries is electric cars.

Table 2-2 summarizes the characteristics of lithium-ion batteries with different cathode materials. The table describes the specification for four most commonly used lithium-ion batteries.

Table 2-2 Specifications of Li-ion batteries with different cathodes (Buchman 2013)

Specifications	**$LiCoO_2$ (LCO)**	**$LiMn_2O_4$ (LMO)**	**$LiFePO_4$ (LFP)**	**$LiNiMnCoO_2$ (NMC)**	**$LiNiCoAlO_2$ (NCA)**
Voltage	3.7V	3.8V	3.3V	3.6V	3.6V
Cycle life	500-1000		1000-2000		
Specific energy Wh/kg	150-190	100-135	90-120	140-180	150-190
Specific rate	1C	10C, 40C	35C	10C	15C
Specific capacity mAh/g	140-150	100-120	150-170	160-170	180-200
Operating temperature	Average	Average	High	High	High
Safety	Requires protection circuit and cell balancing				
Cost	High	Moderate	High	High	High
Notes	Very high specific energy; limited power	Good to high specific energy; high power	Average specific energy; high power	Very high specific energy; high power	Very high specific energy; high power
Applications	Cell phones, laptops	Power tools, medical, EVs	Power tools, auto industry	Power tools, medical, EVs	Electric power train, grid storage

As described in lithium-based batteries, the choice of a cathode provides particular characteristics. Common cathode materials in lithium-ion batteries include lithium cobalt oxide (LCO), lithium manganese oxide (LMO), lithium iron phosphate (LFP), lithium nickel manganese cobalt oxide (NMC), and lithium nickel cobalt aluminum oxide (NCA). The anode in most lithium-ion batteries consists of graphite (Long 2011, Antti and Justin 2012). The global market of lithium-ion batteries has been growing significantly in recent years. The market forecast of lithium-ion batteries for specific applications is listed in Table 2-3 (Gagliardi 2014). Table 2-4 specifies the global market for different types of lithium-ion batteries (Consultants 2013, Gagliardi 2014). The satellite and laptop applications selected for investigation in the present utilize NMC batteries, which are forecasted at the highest volume.

Table 2-3 Li-ion battery application market forecast (‘000 tons)

Applications	2015	2020
Hybrid electric vehicle	6.2	13.8
Plug-in hybrid electric vehicle	6.3	39.7
Electric vehicle	25.3	31.7
Electric bikes	0.3	3.2
Net-books	11.3	24.1
Note-books	29.4	42.0
Mobile phones	22	39.0
Power tools	5.9	8.8
Energy storage system	4.2	18.7
Total	110.9	220.9

Table 2-4 Li-ion battery technology market forecast (‘000 tons)

Technology	2015	2020
NMC	42.9	78.1
LMO	18.0	36.3
LFP	9.2	40.9
NCA	7.9	12.8
LCO	32.9	52.9
Total	110.9	220.9

2.4.5. Manufacturing Process of Lithium-ion Batteries

In this section the manufacturing of lithium nickel manganese cobalt oxide (NMC) batteries are studied. Manufacture of the lithium-ion cell starts with the production of cathodes and anodes, using similar processes (see Figure 2-3). The anode and cathode materials are thoroughly mixed separately in automated mixers to form highly uniform ink-like slurry (Wang, Travas-Sejdic et al. 2002, Ramadass, Haran et al. 2003, Marks, Trussler et al. 2011, Zheng, Li et al. 2012). To make cathodes, the active materials (e.g., NMC) are mixed with Polyvinylidene Fluoride (PVDF) and N-Methyl-2-Pyrrolidone (NMP) and carbon black to make a cathode paste. The polymeric binders such as PVDF and NMP are used to ensure of proper paste adhering during the coating process. Conductive additives e.g., carbon black are required because most transition metal oxide cathode materials have very poor electronic conductivity. The cathode paste is coated onto an aluminum foil which serves as current collector. In contrast, the paste (graphite and the binder) is coated onto a copper foil current collector for anodes. The foils are then dried, pressed to the desired thickness and density, and cut to the proper size before they are wound or stacked, and inserted into the battery cell container. The cells are then filled with the electrolyte and sealed. Following this, the sealed cells are put through the forming process, in which they are charged and discharged 2 or 3 times. Forming step is the longest manufacturing process of lithium-ion batteries. The formed cells are subjected to quality control before they are shipped (Inc 2014, Inc 2014). From cutting process through sealing process, fabrication of NMC batteries is conducted in an environmentally controlled area.

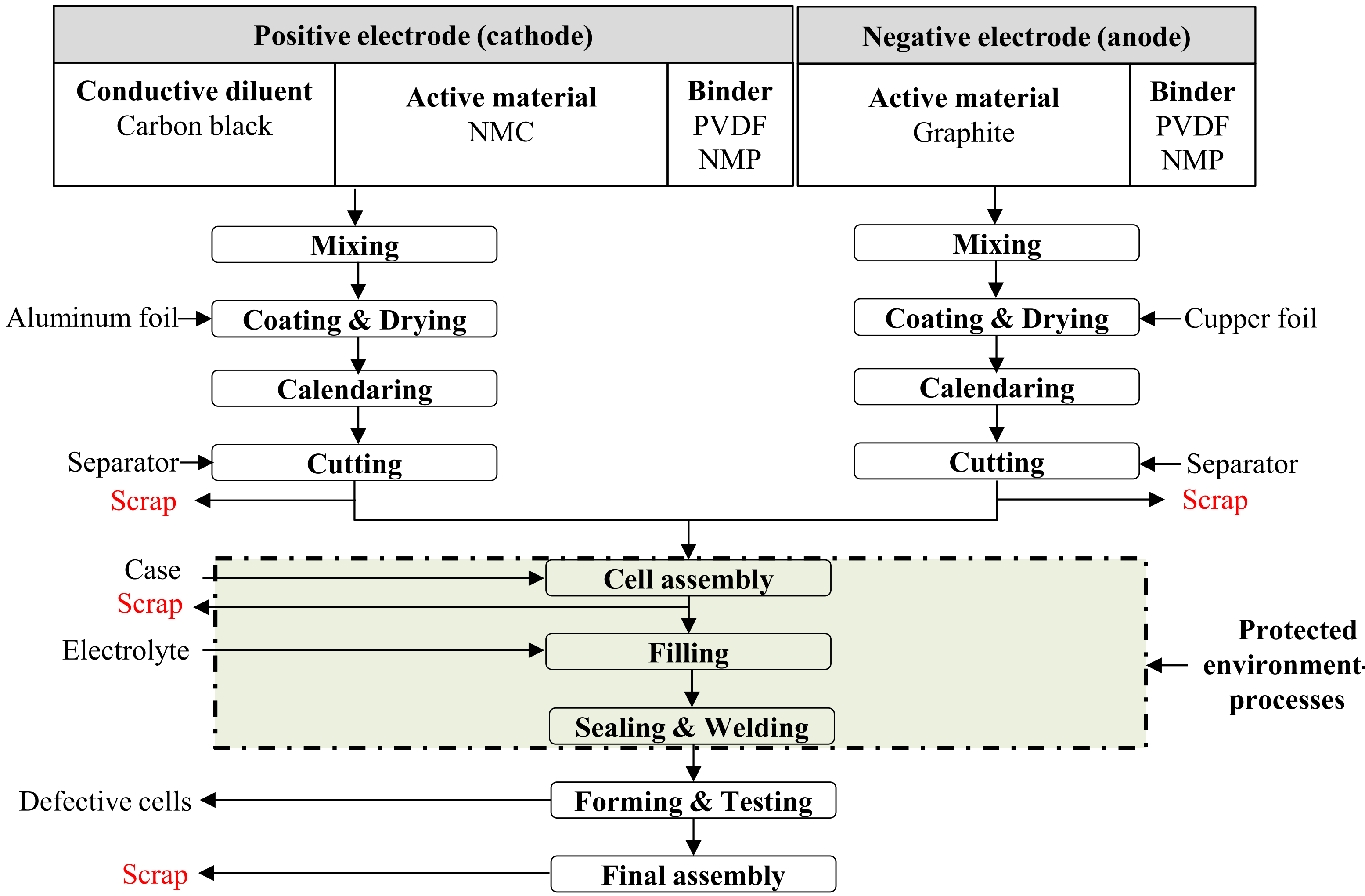


Figure 2-3 NMC battery manufacturing steps (Brodd and Helou 2013)

2.5. CNT Lithium-Ion Batteries

CNTs have great potential for improving the lithium-ion battery performance while they are included as an additive in lithium-ion batteries. As explained in Chapter 1.3 having CNTs in the batteries causes to improve the electronic conductivity of the cathode electrode and increase charge/discharge rate capability of the batteries (Zhang, Cao et al. 2010). Other characteristics which make CNTs desirable for use in lithium-ion batteries include high chemical resistance and low flammability (Jin, Gu et al. 2008). In direct contact with the electrolyte, CNTs in the electrode show high chemical resistance towards an extensive range of organic solvents and lithium-ion salts (Jin, Gu et al. 2008, Song, Park et al. 2011). CNTs may be used for different purposes in different parts of the battery cell, e.g., in cathodes or anodes (Jin, Gu et al. 2008, Chen, Mi et al. 2009, Shanika Amarakoon 2013). In research laboratories, different cathode materials are being developed and tested to create lithium-ion batteries with better performance, longer lifetime, lower thermal tolerance, and higher energy density (Antti and Justin 2012).

This work investigates CNT lithium-ion batteries which are at the research and development stage. These batteries use MWCNT lithium nickel manganese cobalt cathodes and are targeted for satellite and portable computer applications. The anode is made of graphite similar to the anode electrodes in most lithium-ion batteries (Kularatna 2011, Long 2011, Amarakoon 2013). The cell components of CNT NMC battery is shown in Table 2-5.

Table 2-5 Cell configurations of MWCNT NMC battery (Ates, Jia et al. 2014)

Lithium-ion cell / battery part	Material Used
Anode active material	Graphite
Anode substrate	Copper
Cathode active material	MWCNT NMC
Cathode substrate	Aluminum
Separator	Polyethylene
Electrolyte solvent	Organic carbonate and lithium salt

The property improvements in the performance of lithium-ion cells with MWCNTs compared to the performance of the conventional lithium-ion cells in satellites and computers are listed in Table 2-6. To evaluate the benefits of carbon-nanotube-enhanced NMC batteries, versus conventional batteries, two battery systems used in satellites and computers were modeled and compared. Conventional NMC batteries in both applications (satellites and computers) are found in the literature.

A conventional satellite battery which is selected and compared with the newly developed MWCNT NMC battery in this study is used for NASA applications and produced by Yardney Lithion Company (Inc 2014). The battery contains 5 modules with overall 100 lithium-ion cells. The details will be discussed in Chapter 3. For portable computers, the battery which is selected and compared with our product is produced by Panasonic Company. The battery has one module including 6 lithium- ion cells (Inc 2014). The inclusions of CTNs in the battery cell improve many cell parameters including: nominal capacity, specific energy, energy density, power density, and battery life.

Table 2-6 Lithium-ion cells improvement properties with CNTs

Cell Parameters	**Satellites**		**Computers**	
Cell type	**Prismatic**		**Cylindrical**	
Cathode material	NMC	MWCNT NMC	NMC	MWCNT NMC
Anode material	Graphite	Graphite	Graphite	Graphite
Nominal rate	2C	2C	1C	1C
Nominal capacity	25 Ah	30 Ah	1.8 Ah	2.5 Ah
Specific energy	105 Wh/kg	125 Wh/kg	190 Wh/kg	228 Wh/kg
Battery life	2 yrs	4 yrs	3 yrs	6 yrs
Maximum power density	200 W/kg	1800 W/kg	160 W/kg	200 W/kg

The impact of CNTs will vary in satellite and computer battery cells, depending on the amount of CNTs content in the battery active material. The main improvement will occur in the power density of the battery cell in satellites and computers; the increase will be about 800% and 150%, respectively. The battery life in both satellite and computer battery cells will increase by 100%. The other battery cell parameters mentioned in Table 2-6 will improve by around 25% (Ates, Jia et al. 2014, Ates, Mukerjee et al. 2014, Shah, Ates et al. 2014).

2.5.1. Potential hazards of CNT lithium-ion batteries and regulations

As described earlier, there is no clear understanding regarding the impact of nano manufacturing and engineered nanomaterials on human health and the environment (Hischier and Walser 2012). Their exclusive mechanical and chemical properties which make them unique in various applications may also present potential differences in toxicity. Having this difficulty caused to an increase in federal support for nanotechnology toxicology research mainly at the Centers for the Environmental Impacts of Nanotechnology funded by the U.S. Environmental Protection Agency (EPA) (Initiative 2007, Initiative 2008). Also as a precaution, the National Institute for Occupational Safety and Health (NIOSH) suggests handling CNTs and nanoparticles with a hazard-based approach e.g., avoiding exposures (NIOSH 2013). EPA also listed CNTs in the Toxic Substances Control Act (TSCA) inventory (Agency. 2008, NIOSH 2010, Agency 2011). EPA requires documentation, processing notifications, and testing of chemicals to prevent any undesirable environment and human health risks (Agency 2006, Agency October 31, 2008). NIOSH requires the potential exposure of nanoscale materials to be detected and monitored closely in a workplace. The followings are the important things which need to be performed (Musee 2011).

- Developing some methods for measuring the potential exposure of nanoparticles
- Identifying the impacts of the potential release of nanoparticles to the environment
- Identifying the impacts of the potential release of nanoparticles to human health

In addition to measuring the potential exposure of CNTs and carbon nanofibers (CNFs) in a working area, NIOSH also recommends the manufacturing companies to adopt an exposure control strategy and minimize the potential health risks associated with occupational during manufacturing of nanomaterieals (NIOSH 2013). Some of the elements of the NIOSH control plan include:

- Establishing an exposure limit for workers in a workplace (<1 μg/m3 8-hr)
- Having an appropriate worker education and training program
- Installing engineering controls e.g., ventilation system
- Employing a medical surveillance program for workers

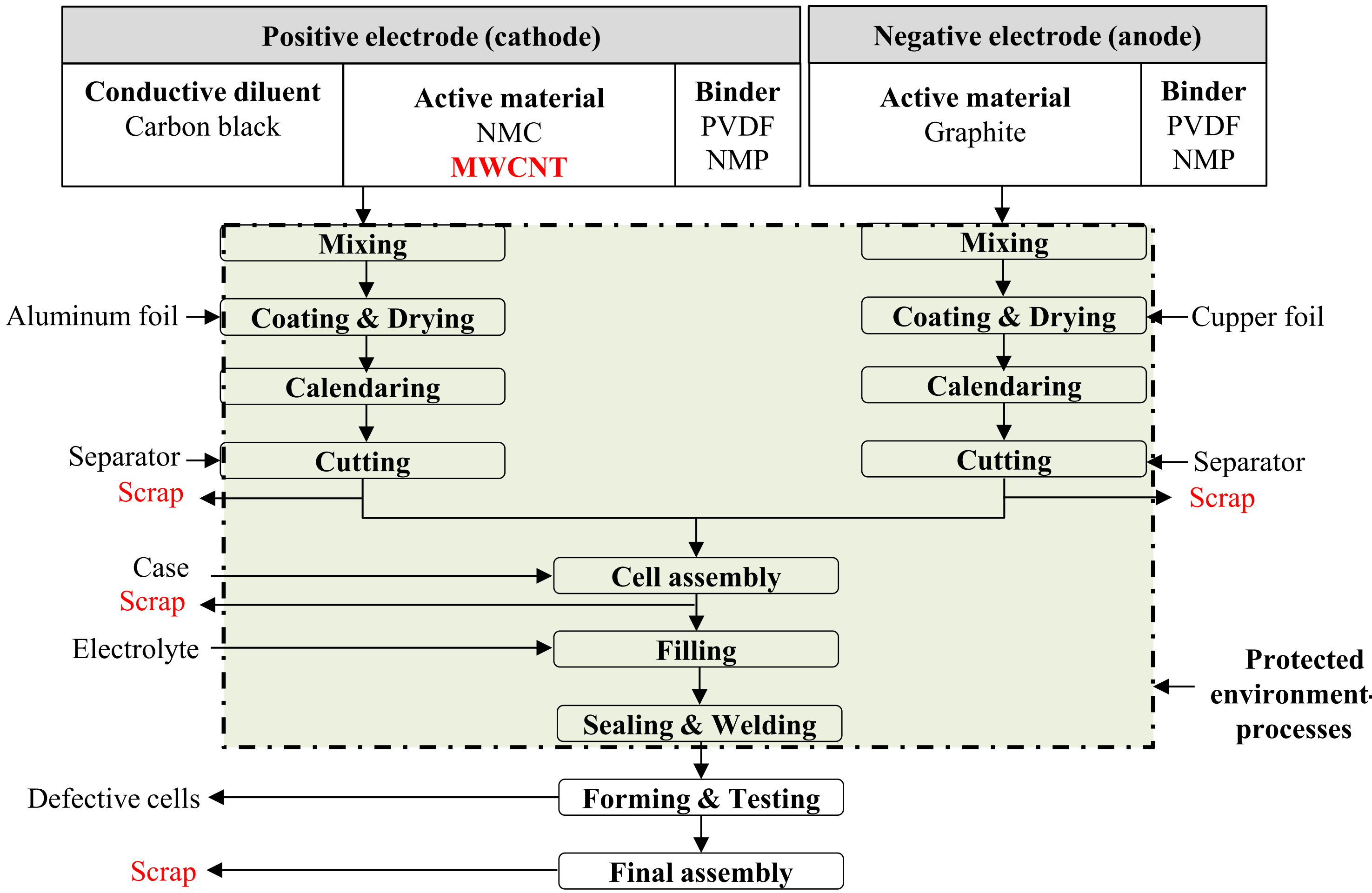


Figure 2-4 Proposed NMC battery manufacturing steps including MWCNT

In this study we developed three different EHS scenarios including low, medium, and high safety standards. The assumptions for each EHS safety standard scenario will be shown in section 3.3. We considered the manufacturing of MWCNT NMC batteries to be conducted in an environmentally controlled area from mixing process (first manufacturing step) through sealing process (Figure 2-4).

In Chapter 3, a process-based technical cost model is described for the manufacturing phase of NMC batteries (Figure 2-5). To construct a cost model, the manufacturing processes, model inputs, physical parameters and assumptions are to be defined. The manufacturing data were collected from a lithium-ion battery manufacturing company located in East Greenwich, Rhode Island. There are various manufacturing process elements that contribute toward total cost individually. The cost effective elements are described in detail and depend upon the elements which are manufactured in certain periods of time. Different environmental health and safety standard scenarios (EHS) are considered. The model has been designed to take into account situations in which the parameters are stochastic. The model also represents the manufacturing unit cost and the total production price range.

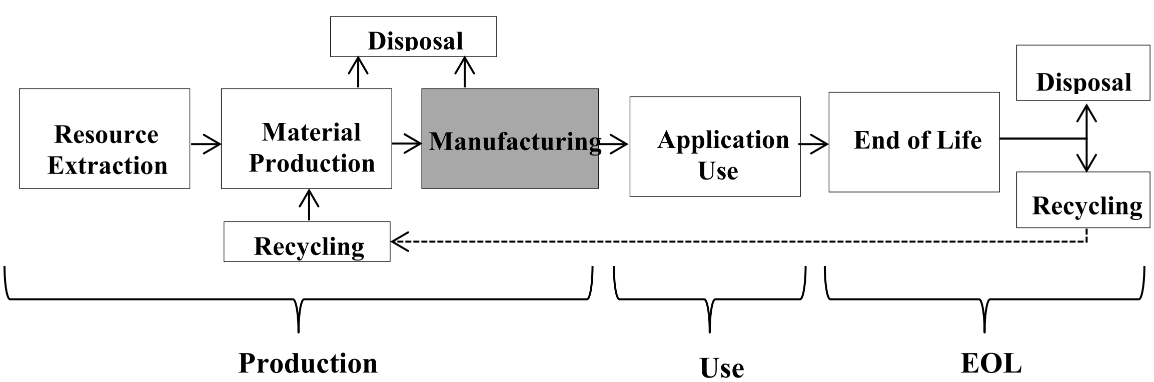


Figure 2-5 Generalized life cycle of products

CHAPTER 3 ECONOMIC ASSESSMENT METHODOLOGY

3.1. Process-based Technical Cost Models

Process-based cost model (PBCM) is a cost estimation tool to assess the manufacturing process costs (Isaacs, Tanwani et al. 2010, Johnson and Kirchain 2010, Nadeau, Kar et al. 2010, P.A. Nelson 2011). This methodology has been used for estimating the product total costs in different manufacturing processes such as SWCNTs and lithium-ion batteries manufacturing for electric-drive vehicles (Locascio 2000, Johnson and Kirchain 2009, Isaacs 2010, P.A. Nelson 2011). Application of PBCM to fabrication processes not only assesses the operational factors of the process, but also enables comparison of alternative materials and processes for products (Johnson and Kirchain 2009, Johnson and Kirchain 2010). After defining individual manufacturing process steps as well as other assumptions and input parameters, the model is programmed to determine the cost differences resulting from changes to base case assumptions. One of the main advantages of applying PBCM methodology is its ability to adapt to the rapid technology turn over and to forecast engineering development costs (Johnson and Kirchain 2010). It is essential for the manufacturers to understand all the cost implications of an emerging technology; to this end, PBCMs offer a means to explore numerous scenarios. For the emerging nanotechnology in batteries, this exploration includes consideration of other critical parameters such as EHS safety standards.

The PBCM methodology and various fixed and variable cost items considered for model development are shown in Figure 3-1. The variable cost parameters are the cost elements which vary in proportion to the total production volume; fixed costs are not affected by the production volume and are one-time capital investments that can be distributed across the entire production volume. In this case, variable costs include material, energy, and labor cost while fixed costs include the cost of equipment, maintenance, building, overhead, and tools (Fuchs, Bruce et al. 2006, Johnson and Kirchain 2010).

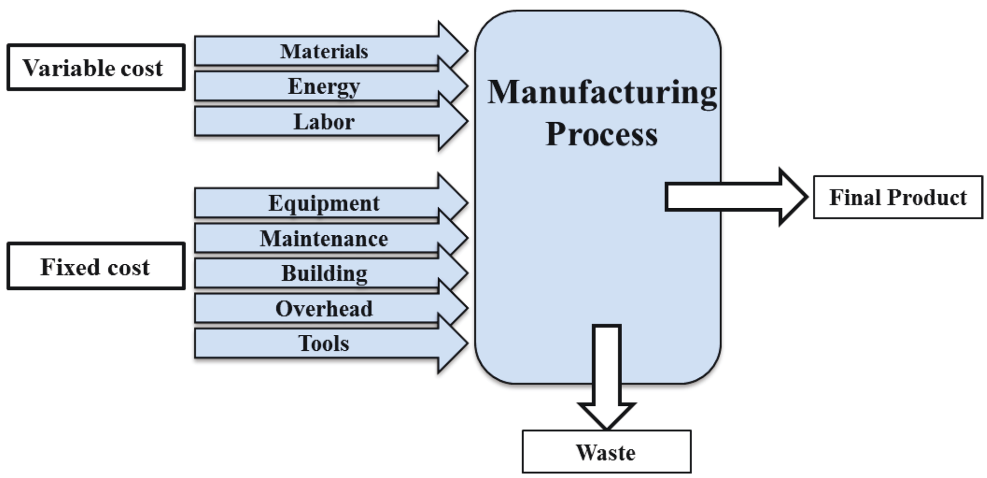


Figure 3-1 Process-based cost modeling tracks the variable and fixed costs of manufacturing

3.2. Model Structure

Application of PBCM to new technologies can inform manufacturers and decision makers about processes which could be improved to make production more economically competitive. We defined the model framework and the process steps for the PBCM for the battery applications. Based on the expected annual production volume, PBCM calculates the required number of the production lines, machines, materials, laborers, and required amount of energy. The corresponding detailed cost and expenses for the resource requirements on each manufacturing process is calculated and projected toward unit cost. The total manufacturing cost per unit is calculated according to the following formulas.

$$\mathrm{C}_U = \frac{\sum_j C_j}{V} \tag{4}$$

where C_U is the cost to produce one unit of product, C_j is the total cost for each cost parameter j (material, labor, energy, equipment, auxiliary equipment, installation, building, tools, overhead, maintenance), and V is the net production volume. The production volume for process step i (V_i) is calculated as :

$$V_i = \frac{V}{Y_i}, \quad \forall i \tag{5}$$

where Y_i is the process yield of the each process step i. By using the production volume for each step i (V_i), total cost for each cost parameter is calculated. For instance, total material cost (C_M) is calculated as follows:

$$C_M = \sum_i V_i \sum_k M_{ik} C_k^M \tag{6}$$

where M_{ik} is the amount of material of type k used in process step i to produce one unit of product, C_k^M is the cost associated with the material type k. Total energy cost (C_E) is calculated as follows:

$$C_E = \sum_i V_i T_i W_i C^E \tag{7}$$

where T_i is the process time in order to produce one product in process step i, W_i is the machine power rate in process step i, and C^E is the energy cost. Total labor cost (C_L) is calculated as follows:

$$C_L = \sum_i (C^{DL} + C^{IL}P)V_iT_i \tag{8}$$

where C^{DL} is the direct labor cost per hour, C^{IL} is the indirect labor cost per hour, and P is the percent indirect labor added on the direct cost.

3.3. Description of Processes and Model Assumptions

Production steps of MWCNT NMC lithium-ion batteries are fashioned after the commercial lithium-ion battery production steps which include electrodes manufacturing, cell assembly, testing, module assembly, and packaging as shown in Figure 2. With the inclusion of CNTs in the process and uncertainty of CNT release, extra safety precautions in the manufacturing facility are recommended (NIOSH 2010, NIOSH 2013). Theses precautionary measures require additional equipment to prevent CNT exposures. A highly controlled environment is therefore continued to enclose the manufacturing steps from mixing to sealing (Figure 2b). The manufacturing process steps of MWCNT NMC batteries and the operating data (Tables 6 & 7) assumed for the model remain consistent for different applications (satellites and computers), but cell specifications and battery part weight percentages (described later) vary for each application. It is assumed that MWCNTs constitute 1% of the total weight of a battery for both satellites and computers. Semi-automated manufacturing processes (one or two workers per fabrication process line) are assumed. Machines can be dedicated or non-dedicated. That means machines can be used to produce either MWCNT NMC batteries only (dedicated) or some other products (non-dedicated).

The manufacturing assumptions data and input parameters for fabricating batteries for three work shifts is shown in Table 3-1 while the assumed cost of main parameters is indicated in Table 3-2 including: labor, energy, and MWCNTs. The average cost of MWCNTs is assumed to be \$600/kg depending on their purities.

Table 3-1 Main assumptions to develop PBCM

Operation Data Assumptions	
Scheduled downtime	1.5 hrs
Hours per day	24 hrs
Days per year	250 days
Building life	30 yrs
Interest rate	10 %
Auxiliary equipment rate*	10 %
Fixed overhead rate*	40 %
Maintenance rate*	5 %
Installation equipment rate*	2 %
Tools rate*	25 %

* % of capital cost

Table 3-2 Parameter cost assumptions

Main Cost Parameter Assumptions	
Energy cost	\$0.15/KWh
Direct labor cost	\$25/hr
Indirect labor cost	\$20/hr
MWCNT cost	\$600/kg
Building cost	\$73/ft^2

As in most manufacturing processes, there will be some defective cells/batteries, i.e., yield is not 100%. Based on the assumed conversion rates and the desired production volume, it is possible to calculate the total amount of scrap during the battery manufacturing. The defective units are collected and sold to the recycling companies. Battery manufacturing companies use the scrap materials as a source of revenue and credit it toward the total unit cost. The recycling companies recover metals such as aluminum, copper, and lithium. It is assumed that there is 5% scrap during the electrode manufacturing and cell assembly, 2% during the final assembly, and 10% scrap during the forming process.

As described in Chapter 2.5.2 National Institute for Occupational Safety and Health (NIOSH) requires the potential exposure of nanoscale materials to be detected and monitored closely in a workplace. In 2013, NIOSH announced the 8-hour time-weighted average (TWA) exposure limit to 1 $\mu g/m^3$ elemental carbon and described the strategies for controlling workplace exposures (Health 2011, NIOSH 2013). In this study, three different EHS scenarios including low, medium, and high safety standards are explored. The assumptions for each EHS safety standard scenario are shown in Table 3-3. A low level EHS standard is assumed to include moderate engineering controls (includes general exhaust ventilation), administrative controls (monthly monitoring), and average personal protective equipment (PPE) requirements (latex gloves, disposal respirators, and Tyvek suits). Medium EHS standards include general as well as local exhaust ventilation. Local exhaust ventilation includes blowers, ductwork, a hood, and a filter. In this scenario, the workplace is monitored for nanoparticle potential exposure once per week. For PPE, workers use nitrile gloves, disposable respirators, and Tyvek suits. High EHS standards include general and local ventilation, biweekly monitoring of workplace, higher levels of PPE, HEPA filter masks instead of disposable respirators; in this standard disposal of PPE is considered as hazardous waste. We consider local ventilation to consist of one blower and two sets of hoods and filters. The ventilation for the clean environment is calculated based on the air change method, where the manufacturing space volume (ft^3) is multiplied by the number of total air changes per hour. The rate of air changes for the manufacturing area is assumed to be 20 changes/hour (Organization 2011).

$$CFM = [Space\ volume\ (ft^3) * air\ change\ rate\ (AC/hr)] /60 \quad (9)$$

Table 3-3 List of assumptions for environmental health and safety (EHS) scenarios

	Level of EHS standards		
Type of EHS control	***Low***	***Medium***	***High***
Engineering controls			
General ventilation	General exhaust ventilation	General exhaust ventilation	General exhaust ventilation
Local exhaust ventilation		-Fume hood -HEPA Filter	-Fume hood -HEPA Filter
Enclosure of processes			Extra equipment
Administrative controls			
Air monitoring	Monthly monitoring	Weekly monitoring	Biweekly monitoring
Medical monitoring			Included
Personal protective equipment			
Gloves	Latex gloves	Nitrile gloves	Nitrile gloves
Respirators	Disposal respirators	Disposal respirators	HEPA filters
Suits		Tyvek suits	Tyvek suits
Disposal of PPE hazardous waste			Included

3.4. Monte Carlo Simulation and Uncertain Parameters

PBCM is modified to work as a Monte Carlo simulation model to account for the uncertain conditions in the battery manufacturing industry (Figure 3-2). By using the Monte Carlo simulation technique, average cost and cost intervals for producing MWCNT lithium-ion batteries can be calculated by generating values for each uncertain parameter: process yield, energy cost, cycle time of the forming step, MWCNT cost, and the disposal of personal protective equipment (PPE) hazardous waste. Since these parameters have the larger effect on manufacturing unit cost in the battery manufacturing industry, they are considered stochastic parameters in the PCBM model. Triangular distribution is assumed for the parameters such as: process yield, disposal cost of PPE hazardous waste, and the cycle time of the forming step, while normal distribution is assumed for energy cost and MWCNT cost parameters. The distribution assumptions for the stochastic input parameters are summarized as follows:

- Process yield: triangular distribution (80%, 85%, 90%)
- MWCNT cost: normal distribution (600, 100)
- Energy cost: normal distribution (0.15, 0.01)
- Disposal of personal PPE waste cost: triangular distribution (0,8,16)
- Cycle time at forming step: triangular distribution (24, 48, 72)

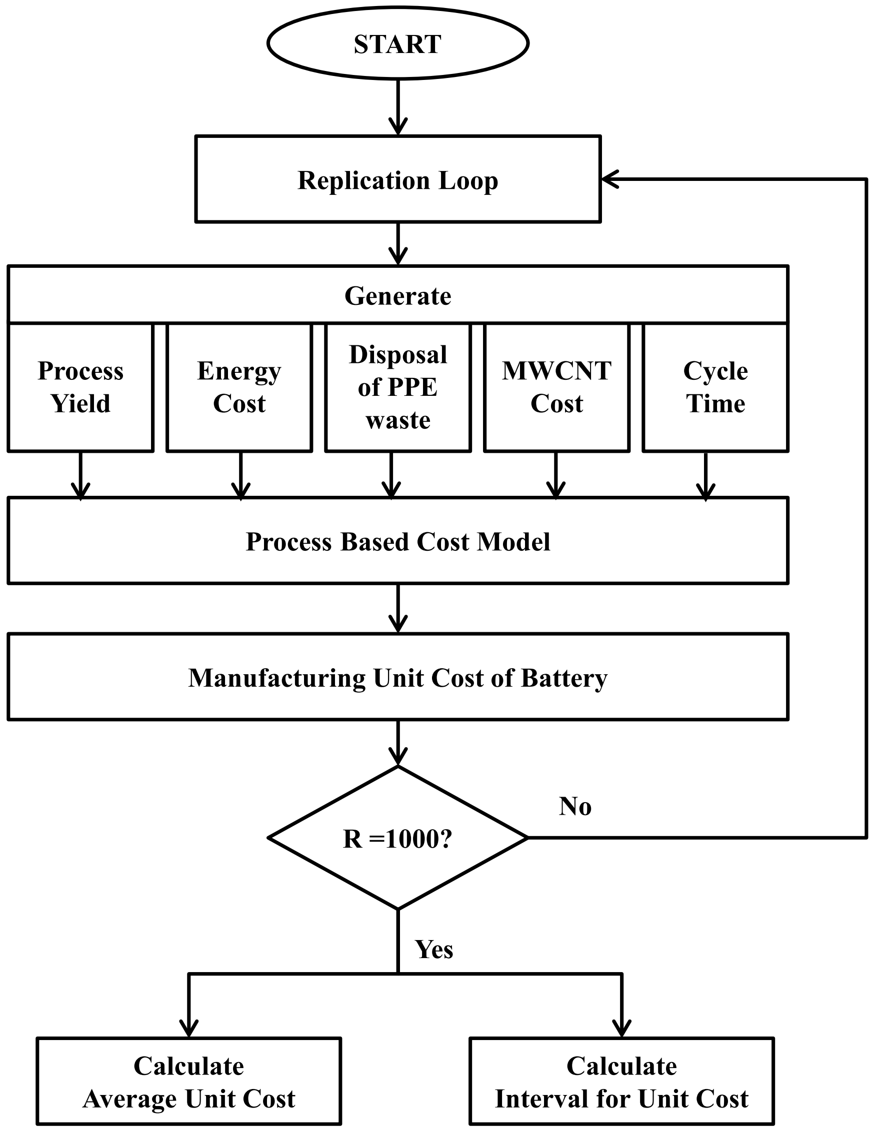


Figure 3-2 Process Flow of Monte Carlo Simulation Model

The simulation model is run 1000 times to calculate the cost ranges. Each time, the MC model generates numbers for the stochastic parameters by using the specified distributions above, and uses these values in the PCBM model to calculate the manufacturing unit cost of the batteries. After running the model 1000 times, the model calculates the average manufacturing unit cost with a 95% confidence interval. In the following section, the results for the modified PBCM model are illustrated.

3.5. Case Studies

In this section, the manufacturing of lithium-ion batteries used in applications such as satellites and portable computers is investigated by applying PBCM methodology.

3.5.1. Satellite Batteries

The key design features of satellite cells are summarized in Table 3-4. The assumptions made regarding the distribution of weights of various CNT battery components are specified in Table 3-5. Each battery contains five modules. Each module contains 20 prismatic cells. While each battery cell weight is 0.908kg, the whole satellite battery weight is 170kg. As mentioned earlier, the forming and testing step takes about 24 to 72 hours depending on the desired battery cycle life. This step makes the cycle time long. It is assumed that the total production volume is 300,000 cells (3,000 batteries) annually. The amount of raw materials, number of production lines, and number of workers are recalculated when the total production volume is revised.

Table 3-4 Satellite CNT Li-ion cell specifications

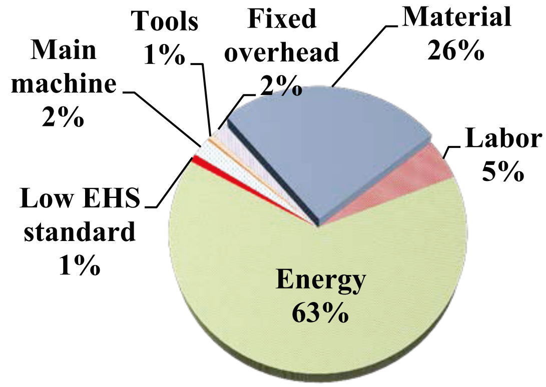
Cell Parameters	**Input Information**
Anode active material	Graphite
Anode substrate	Copper
Cathode active material	MWCNT NMC
Cathode substrate	Aluminum
Separator	Polyethylene
Electrolyte solvent	Organic carbonate & lithium salt
Cell numbers	100 cells in 5 modules
Cell type	Prismatic
Cell dimension	95 mm w *140 mm ht * 28 mm thickness
Nominal cell weight	0.908 kg
Life cycle	> 800 cycles
Nominal rate	30Ah
Nominal voltage	3.6 VDC
Specific energy	125 Wh/kg
Maximum power density	1800 W/kg

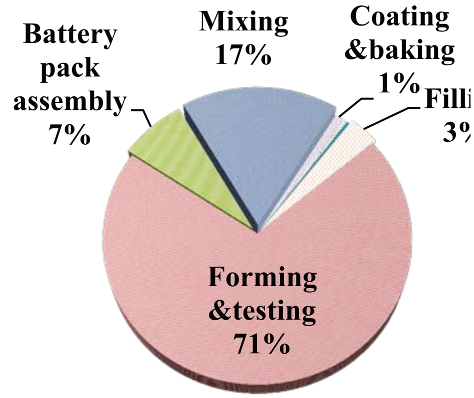
Table 3-5 Satellite battery weight %

CNT Li-ion Battery	**Ranges for Part Weight (%)***	**Specific Input Assumptions**
Anode material	12-18%	15%
Anode current collector	2-5%	3%
Cathode material	20-25%	22%
Cathode current collector	1-3%	1%
Electrolyte	8-12%	10%
Separator	2-4%	2%
Cell container	1-3%	1%
Module container	8-12%	10%
Pack container and battery management systems	30-40%	36%

* (Notter, Gauch et al. 2010, Amarakoon 2013)

In this section, the results obtained from modified PBCM with Monte Carlo simulation for base case (low EHS safety standard option) are discussed. The main cost drivers of manufacturing of lithium-ion batteries are energy cost, cycle time of forming step, material cost, process yield, and disposal of PPE hazardous waste. These parameters are selected as stochastic parameters to calculate the average cost of MWCNT NMC battery for both satellites and computers. The following results were obtained by running the stochastic PBCM model with base case assumptions.





(a) Fixed and variable cost division (b) Cost by production step

Figure 3-3 Manufacturing cost breakdowns of low EHS base case for satellite batteries for mean value

Figure 3-3a and Figure 3-3b illustrate the results by breaking the average cost down for fixed and variable costs and the process steps of manufacturing processes of MWCNT NMC batteries for satellites, respectively. As shown in Figure 3-3a, the fabrication cost of MWCNT lithium-ion batteries is dominated by energy (63%) followed by material cost (26%) and labor cost (5%). Figure 3-3b indicates that the forming and testing step is the highest cost driving step among all the manufacturing steps (71% of the manufacturing unit cost) due to the high energy consumption in forming and testing step.

Mixing step has the second highest impact on the manufacturing unit cost (17% of the manufacturing unit cost) due to use of MWCNTs and the other raw materials in the mixing step. By assuming the total production volume of 300,000 battery cells (3,000 batteries) per year and 10% defective rate in forming and testing step, the average yearly manufacturing of MWCNT NMC batteries for the base case results in a cost of almost $13,486 per satellite battery without considering manufacturing scrap revenue.

The manufacturing waste is assumed to be collected and sold to the recycling companies. The revenue from scrap produced during the manufacturing processes of CNT lithium-ion batteries is calculated based on the total production volume. As discussed in section 3.2, 5% scrap is assumed during the electrode manufacturing while there is 10% scrap during the forming process. If the companies prefer to earn revenue from the scrap, the total unit cost will be $13,311. By collecting and selling the scrap, the company can recover almost $175 per unit product, although this is but a fraction of the cost invested.

3.5.2. Computer Batteries

Table 3-6 describes the specifications of CNT lithium-ion cells in batteries designed for computers. The battery consists of one module which has 6 cells. Unlike satellite battery cells, computer battery cells are cylindrical and much lighter. The weight of each cell is 0.048 kg with a total battery weight of about 0.41 kg. The distribution of the weight of computer battery parts is shown in Table 3-7.

Just as in case of the satellite batteries, the amount of raw materials, number of machines, and number of workers change proportional to the total production volume. Because there is forecasted demand for lithium-ion portable computer batteries in 2018 of 1,000,000 battery units (Espinoza, Erbis et al. 2014), the annual total production volume is assumed to be 1,000,000 batteries.

Table 3-6 Computer CNT Li-ion cell specifications

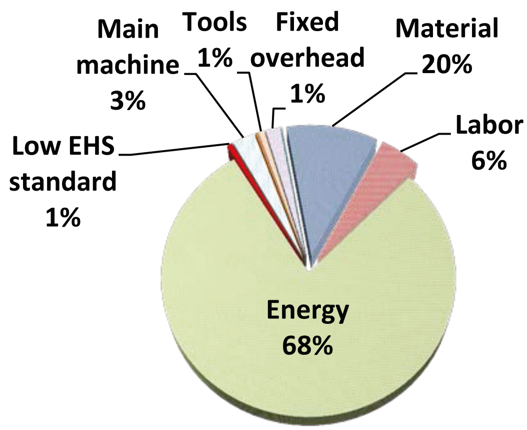
Cell Parameters	Input Information
Anode active material	Graphite
Anode substrate	Copper
Cathode active material	MWCNT NMC
Cathode substrate	Aluminum
Separator	Polyethylene
Electrolyte solvent	Organic carbonate & lithium salt
Cell numbers	6 cells and 1 module
Cell type	Cylindrical
Cell dimension	65.1 mm ht *18.5 mm diameter
Nominal cell weight	0.048 kg
Life cycle	> 800 cycles
Nominal rate	2.5 Ah
Nominal voltage	3.7 VDC
Specific energy	228 Wh/kg
Maximum power density	200 W/kg

Table 3-7 Computer battery weight %

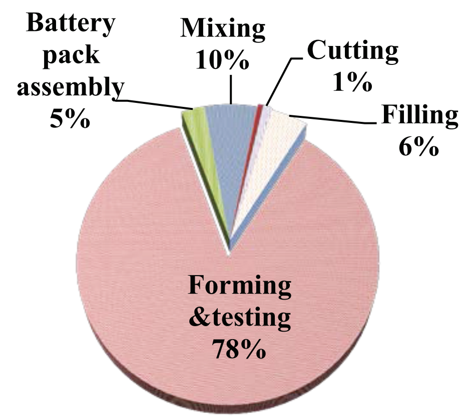
CNT Li-ion Battery	Ranges for Part Weight (%)*	Specific Input Assumptions
Anode material	14-19%	17%
Anode current collector	5-9%	8%
Cathode material	25-30%	25%
Cathode current collector	5-7 %	5%
Electrolyte	10-15%	10%
Separator	2-6%	4%
Cell container	1-3%	1%
Module container	5-10%	5%
Pack container and battery management systems	20-25%	25%

* (Notter, Gauch et al. 2010, Majeau-Bettez, Hawkins et al. 2011)

The cost break down of manufacturing process steps and the variable and fixed costs in computer battery manufacturing are shown in Figure 3-4. Just as in the satellite battery case, energy cost (68% of the manufacturing unit cost) has the highest impact on the manufacturing of MWCNT NMC computer battery unit cost followed by the material cost (20%) and labor cost (6%).



(a) Fixed and variable cost division



(b) Cost by production step

Figure 3-4 Manufacturing cost breakdowns of low EHS base case for portable computer batteries for mean value

As in satellite manufacturing, energy and material cost have greater effect on manufacturing unit cost whereas labor cost has a lower impact on manufacturing unit cost in computer batteries. Because the computer batteries are much smaller than satellite batteries, the material cost percentage is lower for computer battery manufacturing. Figure 3-4b indicates that among the battery production steps, the forming and testing step dominates the total unit cost (78% of the manufacturing unit cost) and has the highest impact on total manufacturing cost. The manufacturing unit cost of MWCNT NMC batteries for computers will be $90 by assuming the annual production volume of 1,000,000 batteries, 10% defective rate in forming and testing step, and low EHS safety standard costs. The manufacturing unit cost decreases minimally (by $1) with credits gained through scrap collection.

3.6. Model Results for Various EHS Scenarios

3.6.1. Satellite Batteries

As mentioned in section 3.2, three different EHS standard scenarios are considered to deal with potential impacts of nanomaterials on human health and the environment. Figure 3-5 shows the variable and fixed cost break down in manufacturing of MWCNT NMC satellite batteries by considering the cost of alternative safety standards. As indicated in Figure 3-5, total manufacturing unit cost comprises 7%, 3%, and 1% for low, medium, high safety standard options, respectively.

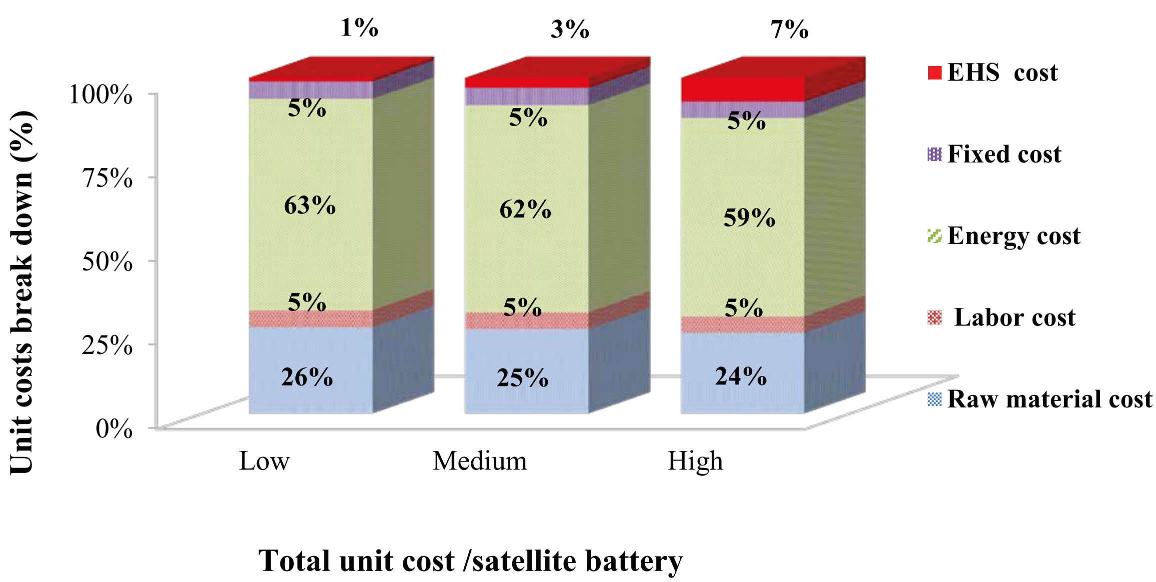


Figure 3-5 Cost break down (EHS cost included) for satellite batteries

After considering the assumptions listed in Table 3-4 and Table 3-5, the amount of waste generated during the process, and the cost of various safety standards, the manufacturing unit cost of CNT NMC batteries (satellites) for different EHS safety options are calculated.

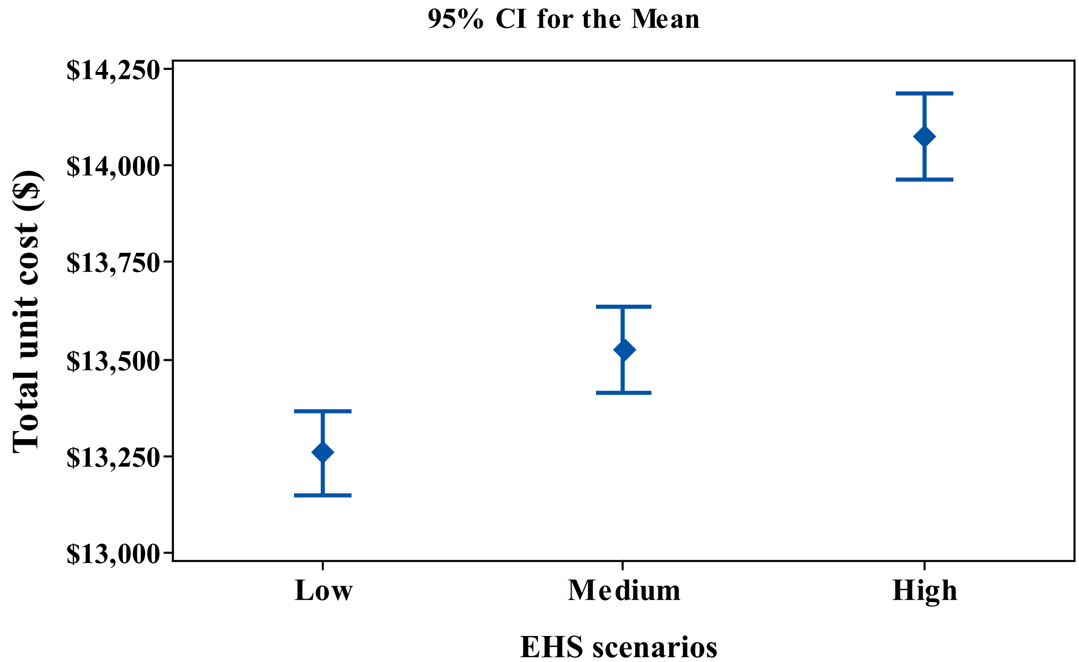


Figure 3-6 Unit cost and confidence intervals of alternative EHS scenarios for manufacture of MWCNT NMC satellite batteries
(Low EHS scenario is reported as base case.)

Figure 3-6 indicates total manufacturing cost intervals for different EHS scenarios. To calculate the average values and intervals for manufacturing unit cost, the simulation model (Figure 3-2) is run for 1000 times by generating numbers for the stochastic parameters. Manufacturing unit cost intervals for different EHS scenarios with 95% confidence interval is determined. The results indicate that if the high EHS standards are preferred or become mandatory in the future, the manufacturing unit cost of battery for satellites with high EHS standards increases by 7% and 5% as compared to low and medium EHS standards, respectively.

As described earlier, the tendency of the total manufacturing unit cost with low, medium, and safety standards is shown in Figure 3-6. To determine the manufacturing cost ranges for different environmental and safety standard scenarios, the histogram charts for each EHS scenario is developed by using Minitab statistical software.

Figure 3-7 shows the total unit cost range for low EHS standard scenario. To calculate the upper and lower manufacturing unit cost, the simulation model (Figure 3-2) is run for 1000 times by generating numbers for the stochastic parameters.

The lower and upper limits of total unit cost in satellite batteries include $8,000 and $17,500, respectively.

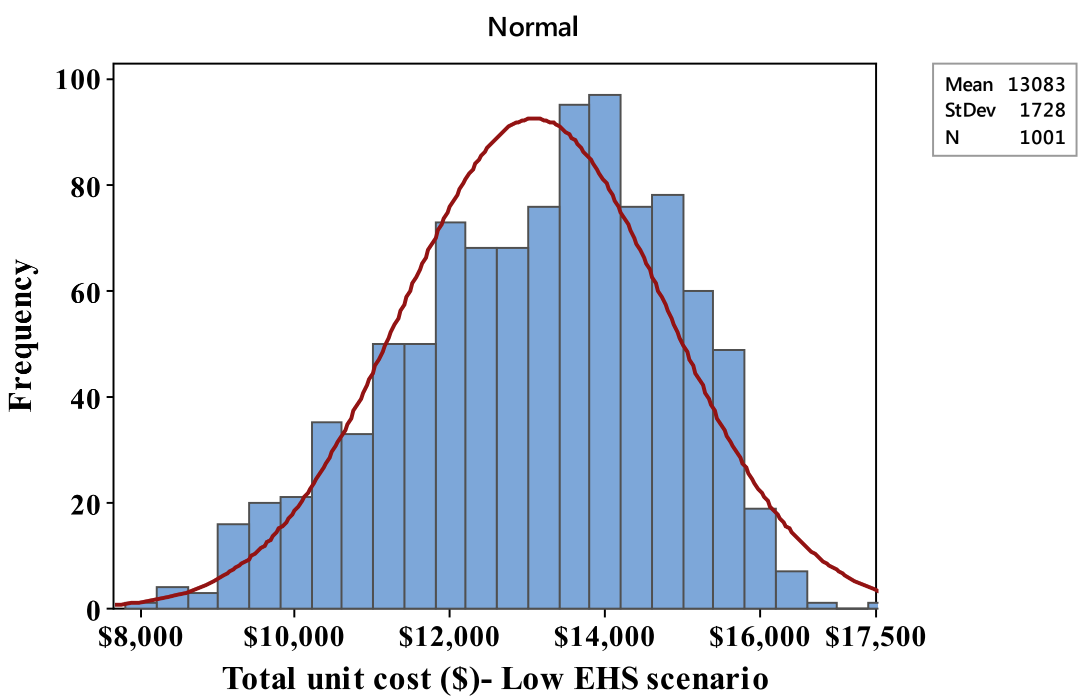


Figure 3-7 Range of total unit cost for low safety scenario for satellite batteries

The range of total manufacturing unit cost including medium safety standards for satellites is shown in Figure 3-8. The lower and upper limits of manufacturing cost of satellite batteries include $8,500 and $18,500, respectively.

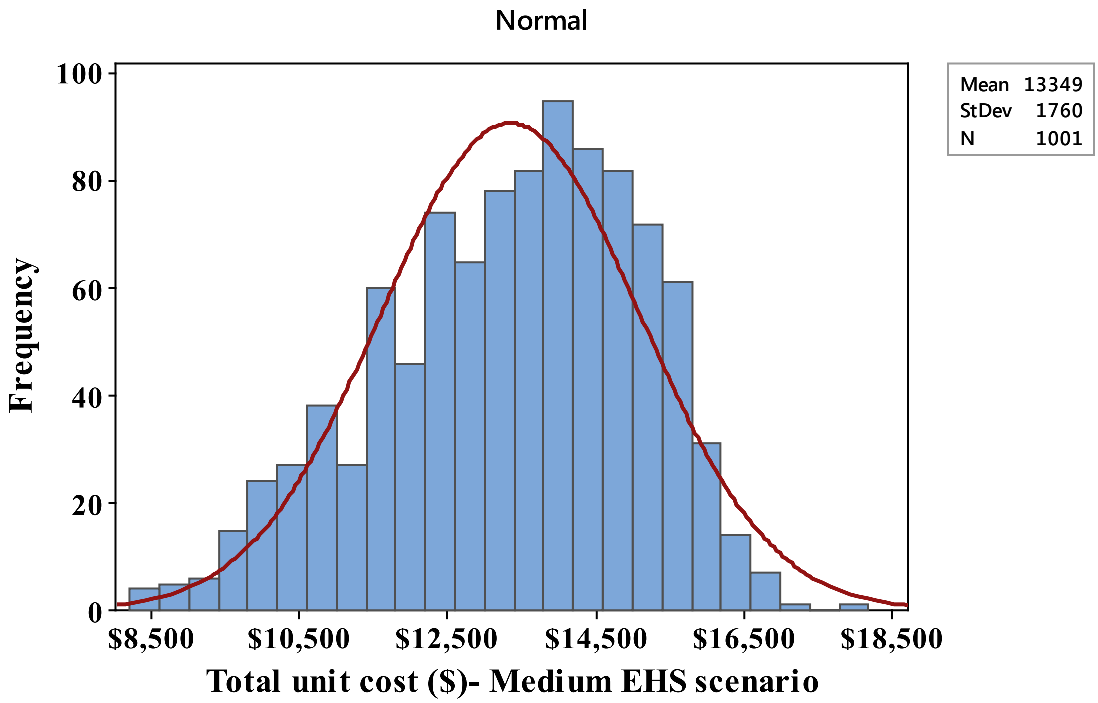


Figure 3-8 Range of total unit cost for medium safety scenario for satellite batteries

Figure 3-9 also indicates the total manufacturing cost ranges for satellite batteries considering high EHS standards by running the simulation model (Figure 3-2) for 1000 times. The upper and lower limits of manufacturing are shown Figure 3-9.

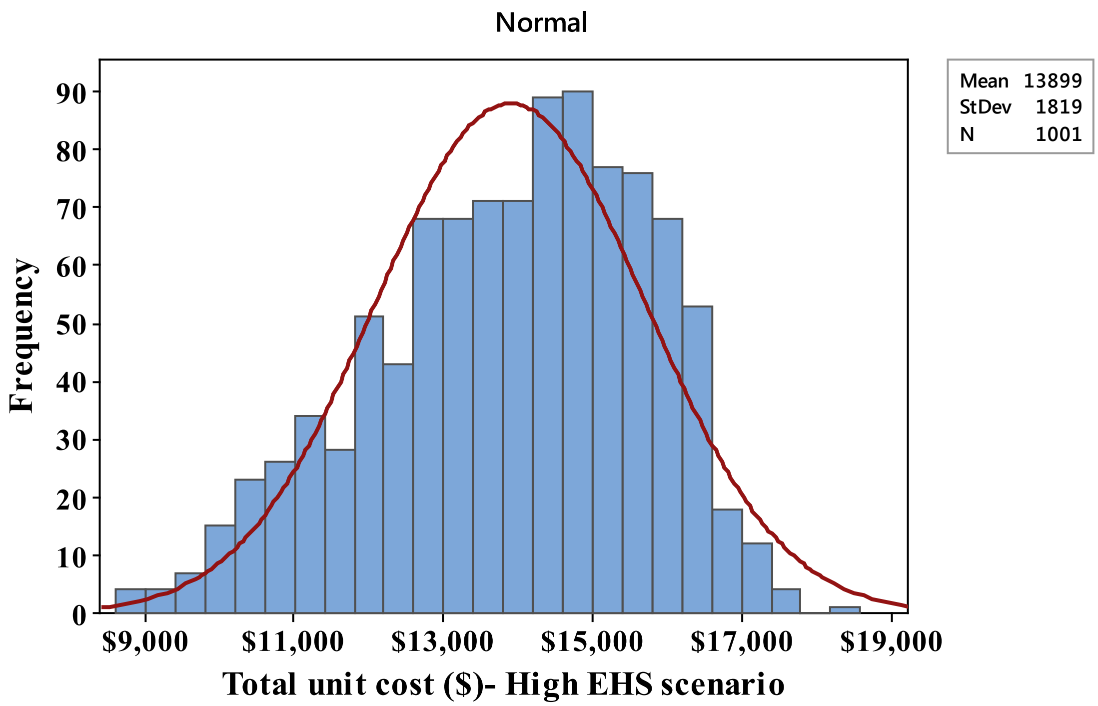
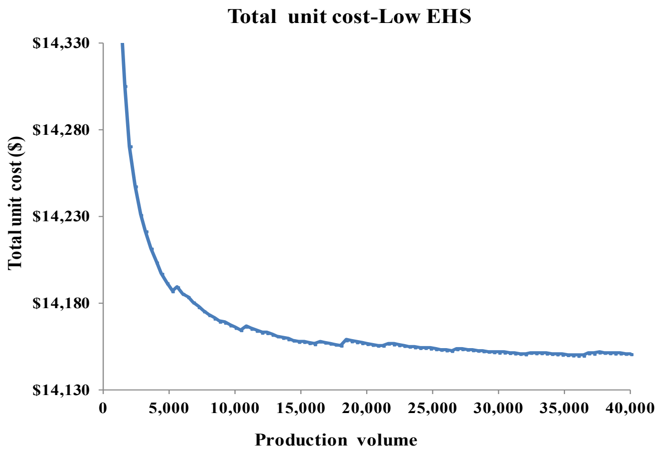
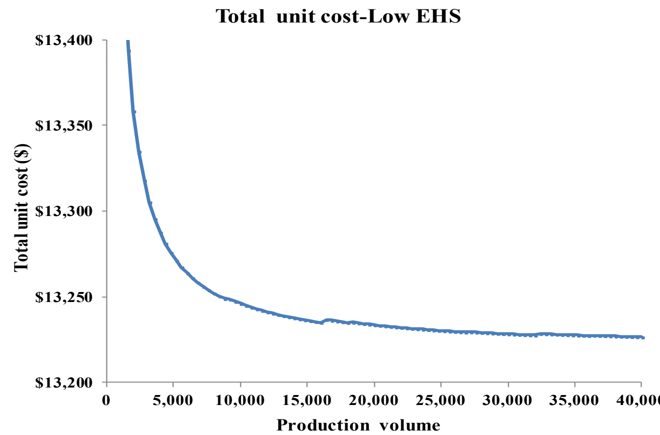


Figure 3-9 Range of total unit cost for high safety scenario for satellite batteries

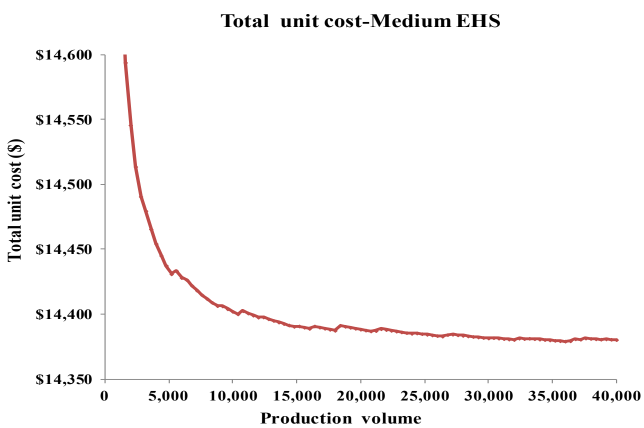
Further analysis was performed using total manufacturing unit costs for different EHS standard scenarios versus total production volume to show the cost fluctuation. The analysis was run for the production rate of 8 and 24 hrs/day. The effect of increasing the production hours per day from 8 to 24 hours for different EHS scenarios (low, medium, and high) are shown in Figure 3-10. The x-axis reflects the production volume range from 0 to 40,000 satellite batteries per year and y-axis shows the corresponding cost per unit for each EHS safety standard. Figure 3-10 indicates the manufacturing total unit cost of satellite batteries including various safety standards decreases while production volume increases. Also Figure 3-10 shows the fluctuation of total manufacturing unit cost while total production volume increases.



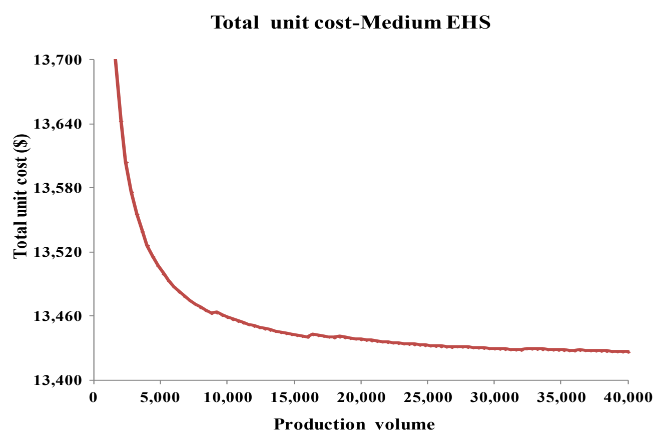
(a): 8h r/day



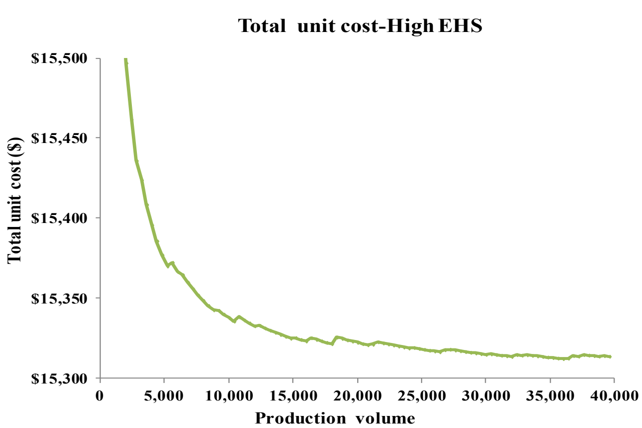
(b): 24 hr/ day



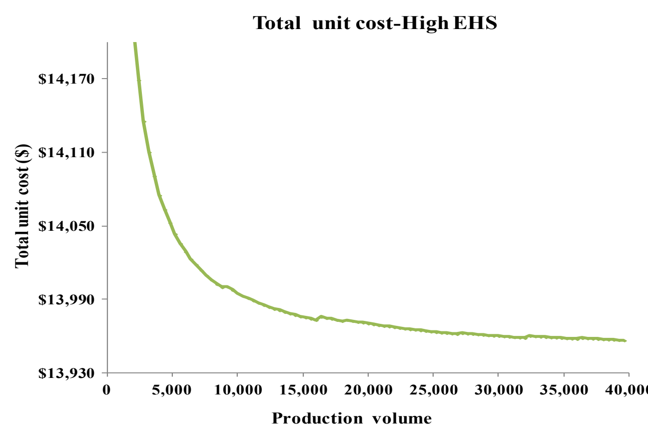
(c): 8hr/day



(d): 24hr/day



(e): 8hr/day



(f): 24hr/day

Figure 3-10 Total unit cost of different EHS scenarios vs. production volume for different production rates for satellite batteries

To determine the causes of unit cost fluctuation during manufacturing of batteries, fixed and variable cost parameters with respect to production volume are studied. The study is developed for production rates of 8 and 24 hrs per day, respectively. Figure 3-11a and Figure 3-11b show the corresponding fixed costs of different production volume for production rate of 8 and 24 hours per day while Figure 3-11c and Figure 3-11d show the corresponding variable costs of various production volumes. Figure 3-11 indicates the cause of manufacturing unit cost fluctuation is the variation of fixed cost parameters because variable costs remain constant when the production volume changes.

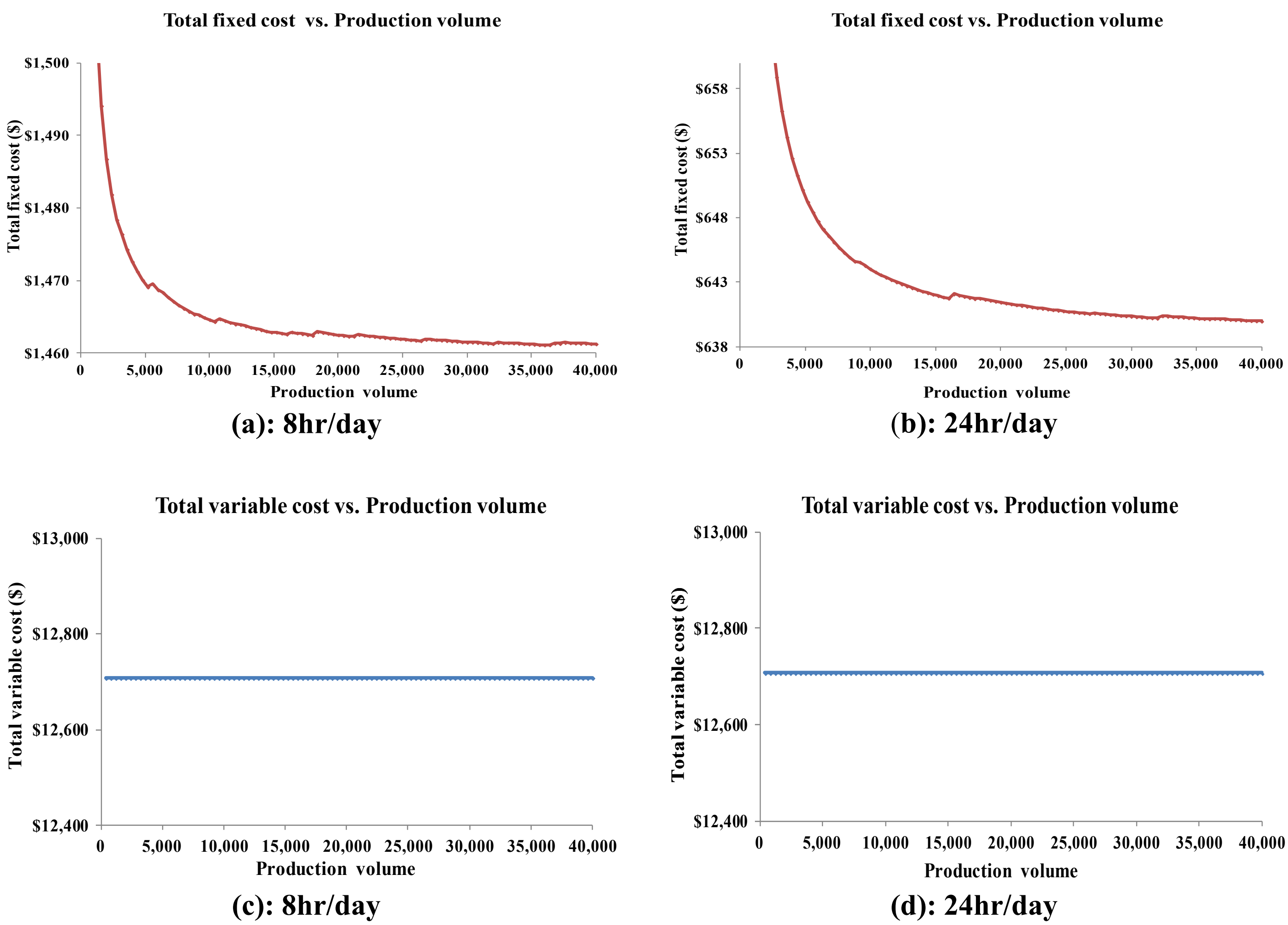


Figure 3-11 Total fixed and variable costs vs. production volume for different production rates for satellite batteries

Figure 3-12 shows the cost variation of different EHS scenarios (low, medium, and high scenarios) in respect with various production volumes for 8 and 24 working hours per day. As shown in Figure 3-12, when the production volume increases, the total EHS cost for different safety scenarios becomes steady.

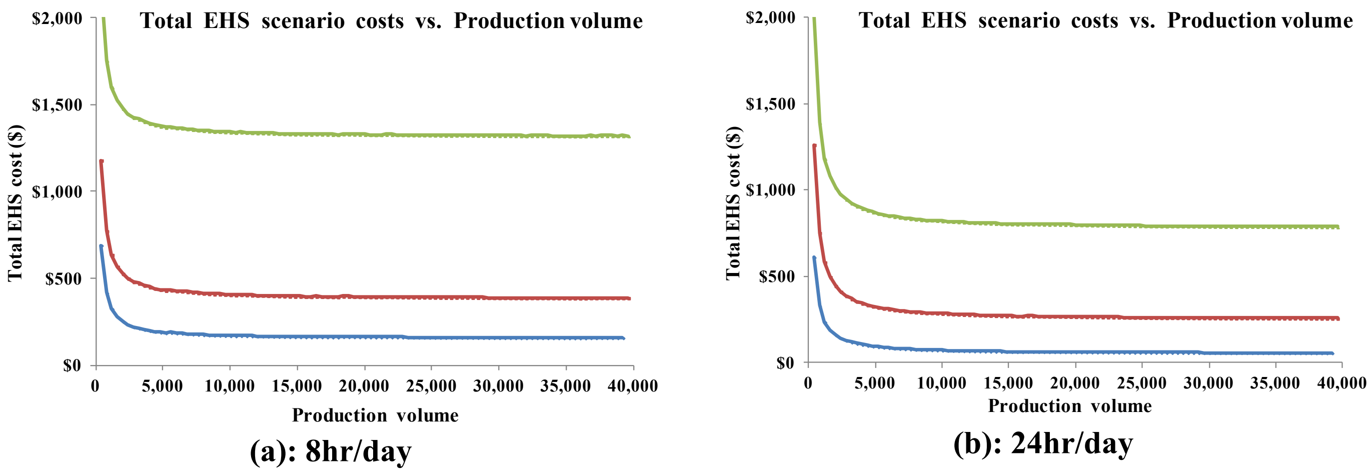


Figure 3-12 Total EHS safety scenario costs vs. production volume for different production rates for satellite batteries

3.6.2. Computer Batteries

As explained, with consideration of different safety standards (low, medium, and high EHS scenarios) in the manufacturing area, fixed and variable cost percentages of total unit production cost are changed. Figure 3-13 shows all the adjusted percentages in details for computer batteries. Choosing high EHS safety standards in the manufacturing area resulted in higher total unit compared to low and medium EHS standards by 6% and 4%, respectively. 7% of total manufacturing cost includes the cost of having high safety standards in the manufacturing area while having medium or low safety standard option during MWCNT NMC batteries for computers includes 3% and 1% of total manufacturing cost, respectively.

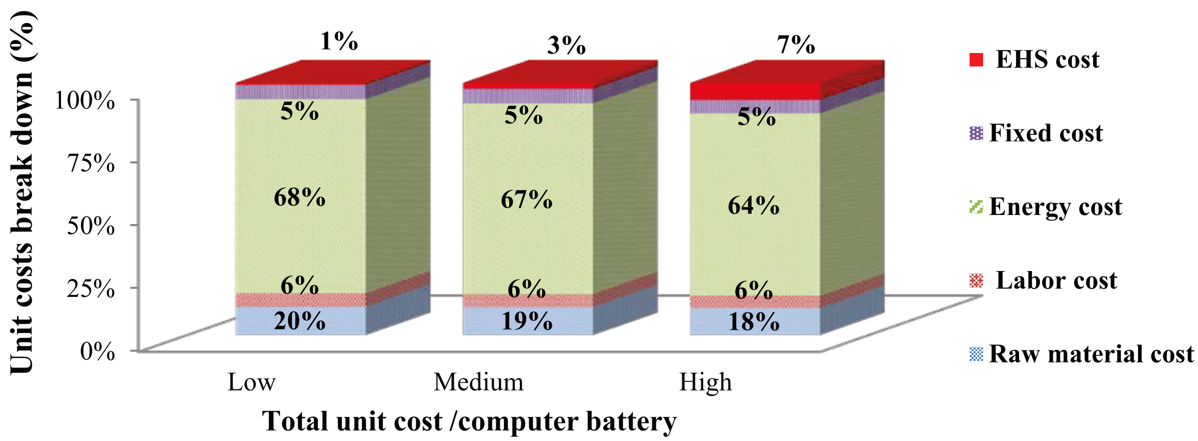
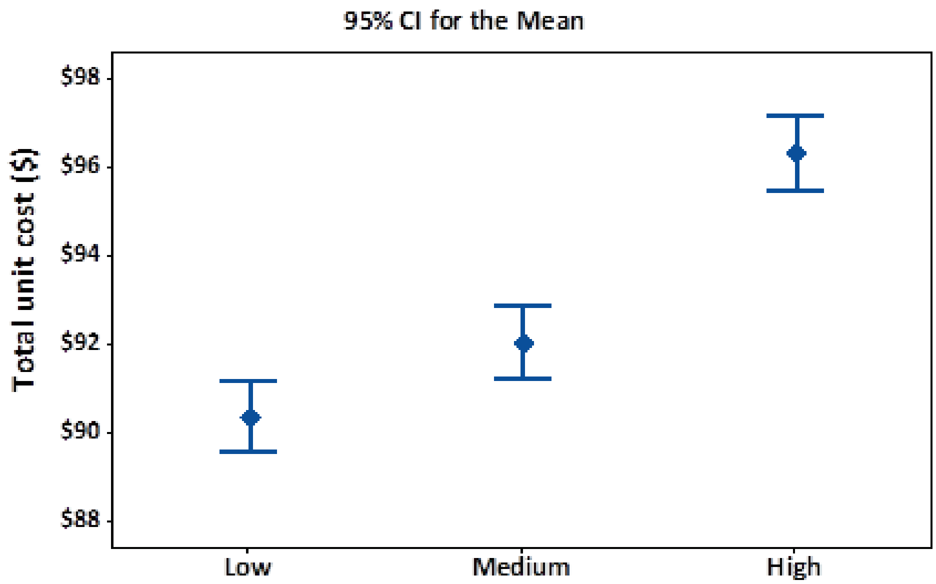


Figure 3-13 Cost break down (EHS cost included) for computer batteries

Figure 3-14 shows the cost confidence intervals of manufacturing unit cost of MWCNTs lithium-ion batteries for computers. Considering the parameter stochasticity, the manufacturing assumption listed in Table 3-6 and Table 3-7, and different EHS scenarios, mean value of manufacturing unit cost (batteries in computers) increases if the companies choose to have safer manufacturing working area. However, the increase in the manufacturing unit cost for computer batteries is smaller than it is for the satellite batteries due to differences in product design.



EHS scenarios

Figure 3-14 Unit cost and confidence intervals of alternative EHS scenarios for manufacture of MWCNT NMC computer batteries
(Low EHS scenario is reported as base case.)

As indicated earlier, total manufacturing unit cost tendency and cost intervals for different EHS scenarios was shown in Figure 3-14. Likewise in satellite batteries, to determine the manufacturing cost ranges of computer batteries including different safety standard options, the histogram charts for each EHS scenario is developed. First, the simulation model (Figure 3-2) is run for 1000 times for each EHS standard option. By using the Minitab analysis software, the unit cost ranges for different safety scenarios is calculated. Figure 3-15 shows the total unit cost ranges for low EHS standard scenario for computer batteries. As shown in Figure 3-15, total unit cost of computer batteries including low EHS standard varies between $51 (lower limit) and $131 (upper limit).

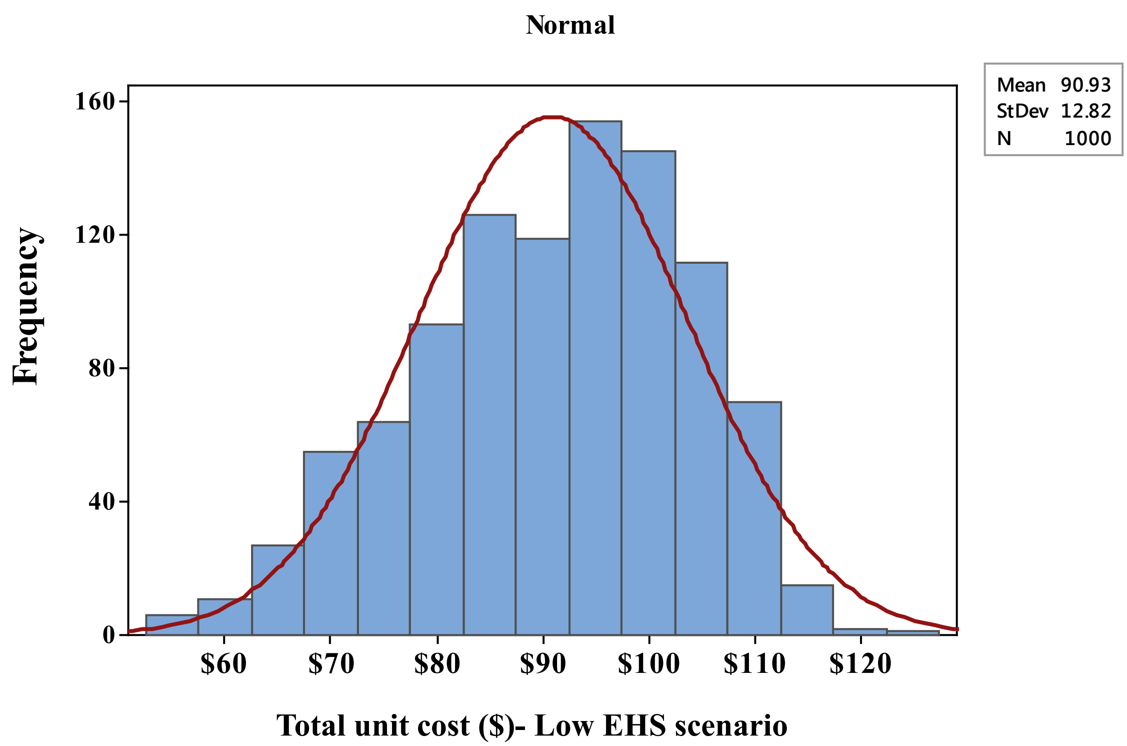


Figure 3-15 Range of total unit cost for low safety scenario for computer batteries

The range of total manufacturing unit cost including medium safety standards for satellites is shown in Figure 3-16. The lower and upper limits of manufacturing cost of computer batteries vary between $53 and $134, respectively.

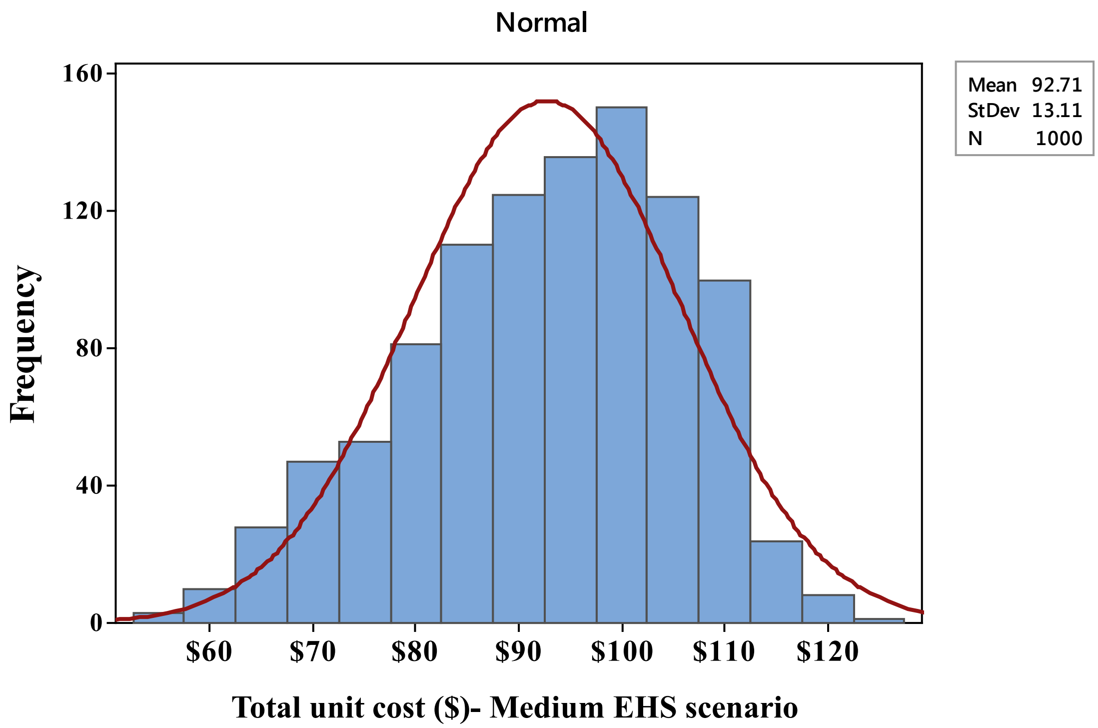


Figure 3-16 Range of total unit cost for medium safety scenario for computer batteries

Figure 3-17 also indicates the total manufacturing cost ranges for satellite batteries considering high EHS standards by running the simulation model (Figure 5) for 1000 times. The upper and lower limits of manufacturing are shown in Figure 3-17 which varies between $57 and $141.

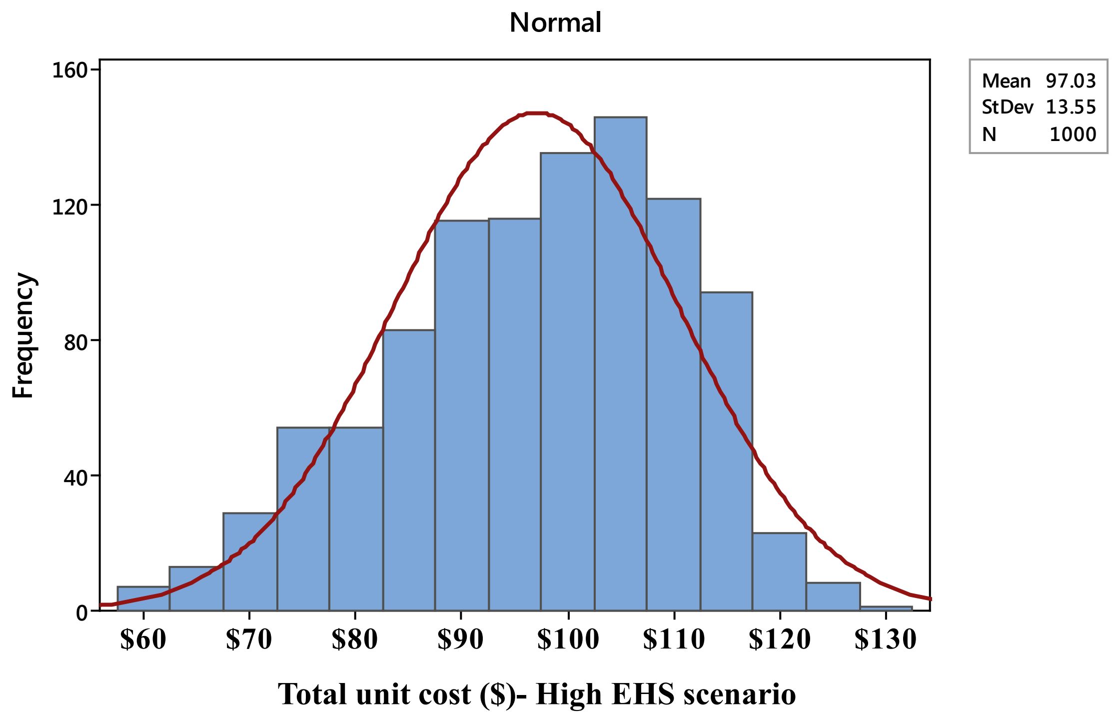


Figure 3-17 Range of total unit cost for high safety scenario for computer batteries

The same analysis in satellite batteries is run for the computer batteries to verify the cause of total cost fluctuation with respect to production volume. As shown in Figure 3-18, by increasing the production volume, the total manufacturing unit cost is decreased until getting to the steady state. The analysis was developed for different EHS scenarios (low, medium, and high) considering the production rate of 8 and 24 hrs/day. Figure 3-18 shows the fluctuation of total manufacturing unit cost while total production volume increases.

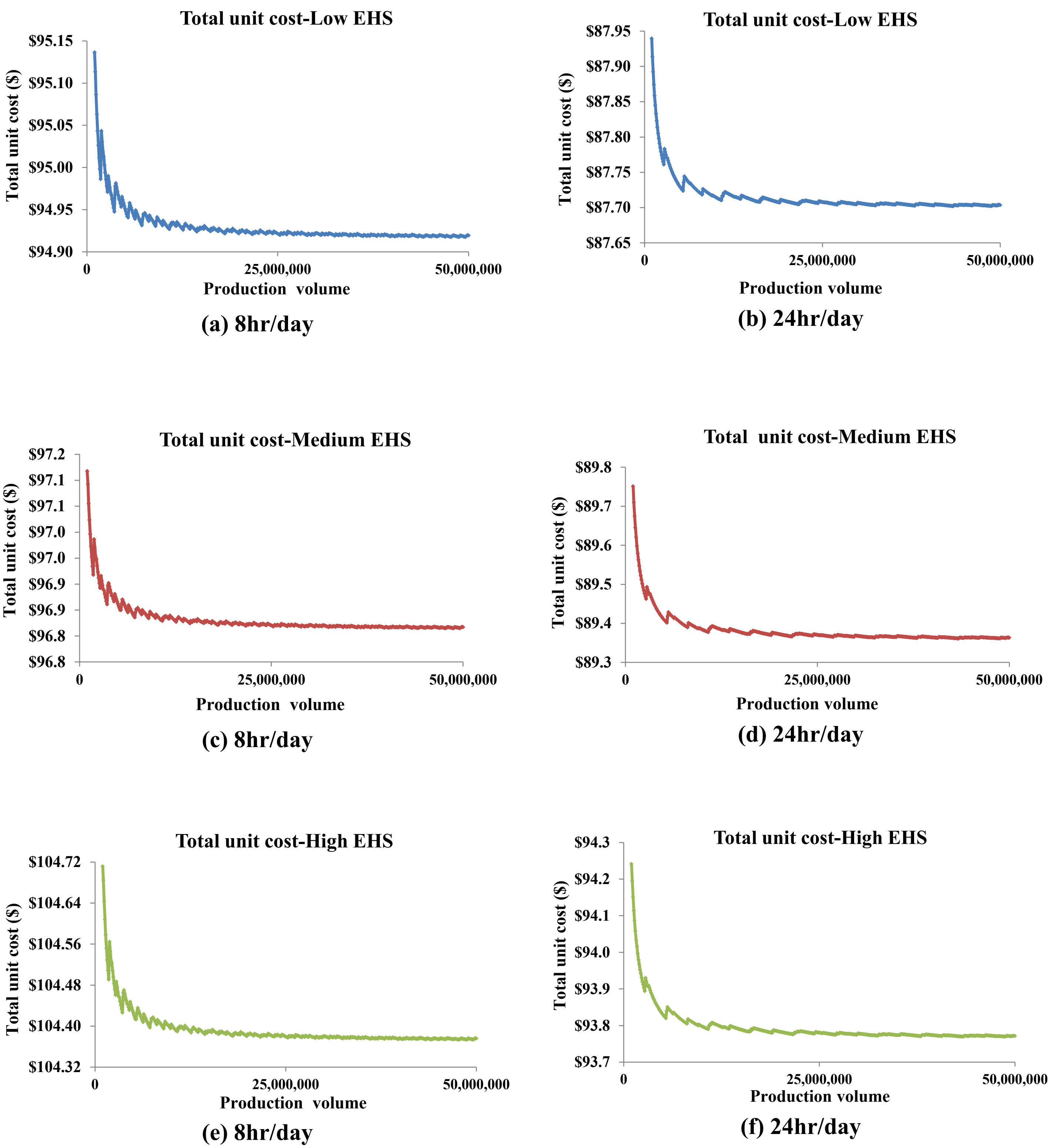
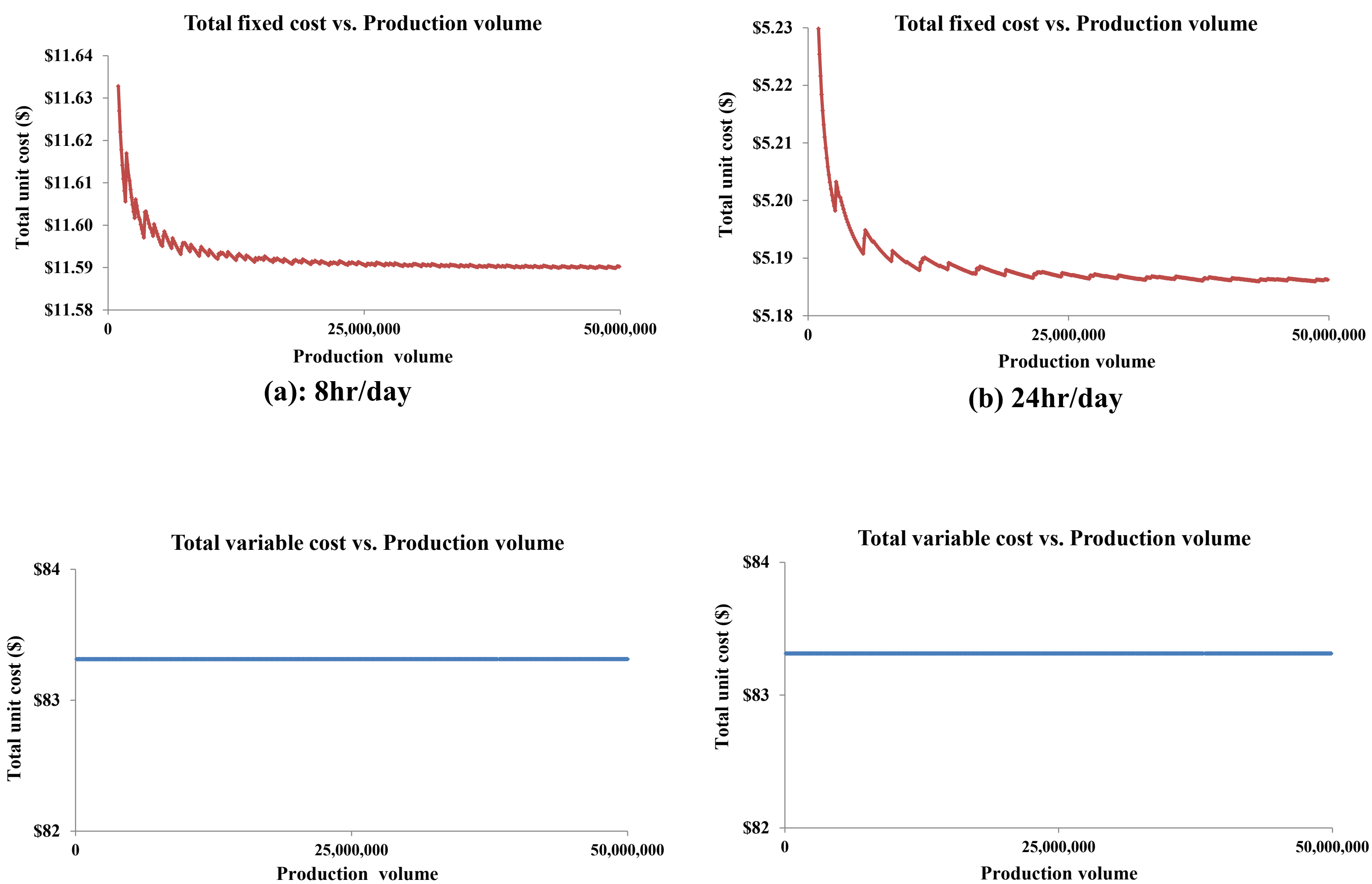


Figure 3-18 Total unit cost of different EHS scenarios vs. production volume for different production rates for computer batteries

Similar to satellites batteries, after studying the fixed and variable cost with respect to production volume in computer batteries, the cause of total unit cost fluctuation is verified. The results indicate the cause of manufacturing unit cost fluctuation is the variation of fixed cost parameters (Figure 3-19a and Figure 3-19b) because variable costs remain constant (Figure 3-19c and Figure 3-19d) when the production volume changes. The analysis was run for 8 and 24 hours working time per day.



(a): 8hr/day

(b) 24hr/day

(c) 8hr/day

(d) 24hr/day

Figure 3-19 Total fixed and variable costs vs. production volume for different production rates for computer batteries

Figure 3-20 shows the cost variation of different EHS scenarios (low, medium, and high scenarios) in respect with various production volumes for 8 and 24 working hours per day. As shown in Figure 3-20, when the production volume increases, the total EHS cost for different safety scenarios decreases until getting into the steady state.

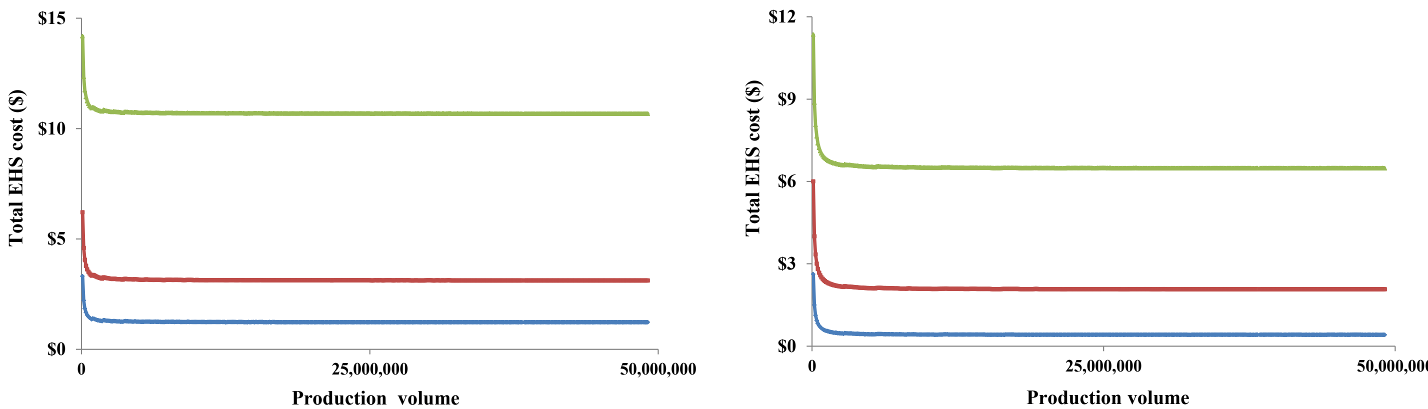


Figure 3-20 Total EHS safety scenario costs vs. production volume for different production rates for computer batteries

3.7. Design of Experiment Results

Experimental design analysis is run in order to investigate the factors which have significant effect on the manufacturing unit cost. Process yield, disposal cost of personal protective equipment (PPE) hazardous waste, cost of MWCNT, energy cost, and cycle time of forming step are the parameters which are selected for the experimental design analysis. The high, low, and base level values for the factors are shown in Table 3-8. These values are used for both satellite and computer batteries. As mentioned before, triangular distributions ([a, c, b]) are used to generate process yield, disposal cost of PPE hazardous waste, and cycle time values whereas normal distributions ($\boldsymbol{\mu}$, σ) are used to generate cost of MWCNT and energy cost values. For each level, different distribution parameters are used to run the experimental design analysis.

Table 3-8 High, low, and base level values for input parameters with triangular distributions for process yield, cycle time and PPE waste cost and normal distributions for energy and MWCNT costs

	Process yield X_1	**MWCNT cost** X_2	**Energy cost** X_3	**PPE waste** X_4	**Cycle time** X_5
1	(0.9,0.95,1)	(800,100)	(0.2,0.01)	(8,16,24)	(60,72,84)
0	(0.8,0.85,0.9)	(600,100)	(0.15,0.01)	(0,8,16)	(24,48,72)
-1	(0.7,0.75,0.8)	(400,100)	(0.1,0.01)	(0,4,8)	(12,24,36)

Main and interaction effect of the factors on manufacturing unit cost of lithium-ion batteries with CNTs are investigated by running full factorial design. A three level design with 5 factors has 243 possible combination treatments. The PBCM model was run for each combination. MINITAB was used to analyze the results.

Figure 3-21 shows the main effects of the factors on manufacturing unit cost for battery used in satellites. Figure 3-21 states cycle time at forming step has more effect on manufacturing unit cost for the satellite batteries than the other factors due to increase in energy consumption at forming step when cycle time is increased. As discussed in section 2, cycle time at forming step is the longest manufacturing process and usually takes between 24 to 72 hours. The factor which has the second most effect on manufacturing unit cost is energy cost. Similar to cycle time at forming step, energy cost has significant effect on manufacturing unit cost of MWCNT NMC batteries used in satellites. If the company chooses to use more expensive energy type such as renewable energy, manufacturing unit cost increases significantly due to high consumption of energy during manufacturing. Unit labor cost has the less effect on manufacturing unit cost than cycle time and energy cost due to the fixed number of labors for each process line. Process yield has negative effect in manufacturing unit cost. If the company invests on better technologies for producing the batteries, the manufacturing unit cost decreases.

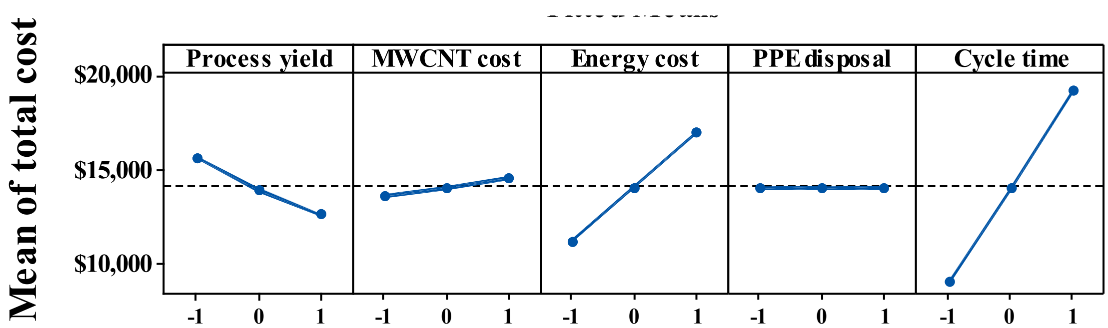


Figure 3-21 Main effects plot diagram for satellite batteries for high EHS scenario at the mid-value level (0)

Figure 3-22 shows the interaction plots for satellite batteries. Interaction plot shows the effect of factor pairs on manufacturing unit cost. As shown in Figure 3-22, the interaction between the energy cost and cycle time has the most effect on manufacturing unit cost among all factor pairs.

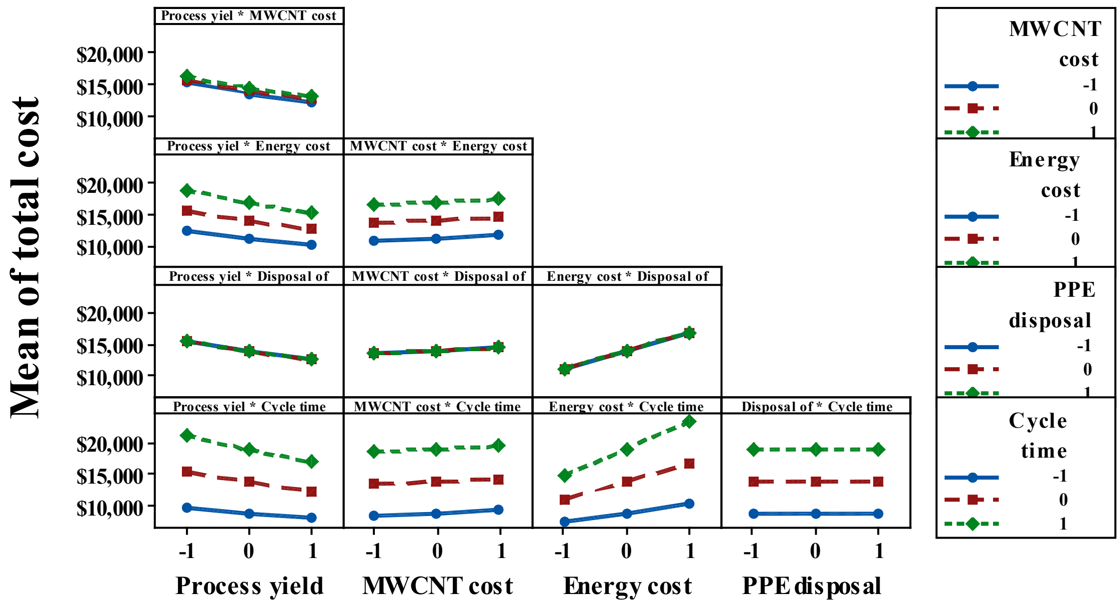


Figure 3-22 Interaction plot diagram for satellite batteries for the high EHS scenario

Response surface graph in Figure 3-23 illustrates the effect of the energy cost and cycle time on manufacturing unit cost. If large cycle times at the forming step and renewable source of energy are preferred during the manufacturing of satellite batteries, the manufacturing cost increases significantly. However, manufacturing unit cost decreases if small cycle times at forming step and low cost energy type are desired during the manufacturing. Since both cycle time at forming step and energy cost have significant effect on manufacturing unit cost of satellite batteries with CNTs, the type of energy used during battery manufacturing and cycle time at forming step should be optimized in order to minimize the manufacturing unit cost by also considering the specification of the new generation satellite battery with CNTs.

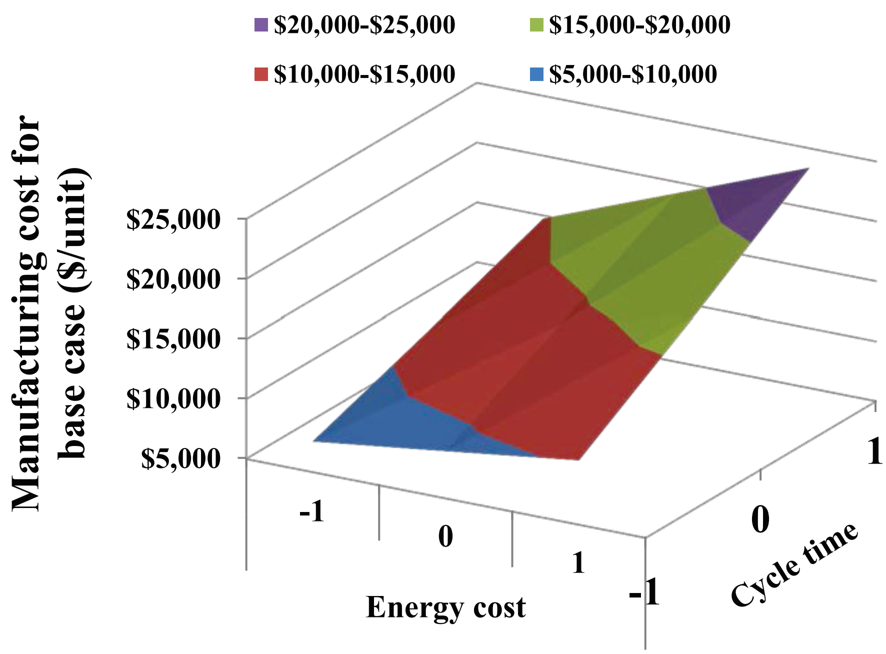


Figure 3-23 Surface graph for satellite MWCNT-enabled batteries for parameters with greatest influence on manufacturing cost, holding all other parameters at base level (0) values (for high EHS scenario)

After identifying the main factors which have the highest impact on the total unit cost and developing the effect of factor pairs on manufacturing unit cost (Figure 3-22), a two-level design with five factors is also considered to generate the standardized effect plot by using Minitab. Table 3-9 shows all the possible combinations. The values in the P column of Table 3-9 are used to determine which of the effects are significant. The alpha value (α) is kept the same at 0.05. The blue highlighted factors in Table 3-9 and Table 3-10 are identified as significant since they have P-values less than 0.05. The T value for the cycle time is higher with a value of 269.16 than the rest of the main effects, meaning that its impact is the highest on the total cost.

Table 3-9 Estimated effects and coefficients for satellite batteries (high EHS)

Term	Effect	Coefficient	SE Coeff	T	P
Constant		14111.7	15.5	911.37	0
Process Yield	**-3077.3**	**-1538.7**	**19.1**	**-80.41**	**0**
MWCNT Cost	**936.2**	**468.1**	**19**	**24.66**	**0**
Energy Cost	**5818.1**	**2909**	**19**	**153.27**	**0**
Disposal of PPE Cost	**69.1**	**34.5**	**19**	**1.82**	**0.07**
Cycle Time	**10203.3**	**5101.6**	**19**	**269.16**	**0**
Process Yield*MWCNT Cost	**-124.7**	**-62.3**	**23.6**	**-2.65**	**0.009**
Process Yield *Energy Cost	**-699.4**	**-349.7**	**23.6**	**-14.84**	**0**
Process Yield* Disposal of PPE Cost	**-17.7**	**-8.9**	**23.6**	**-0.38**	**0.708**
Process Yield *Cycle Time	**-1217.5**	**-608.8**	**23.4**	**-26.05**	**0**
MWCNT Cost *Energy Cost	**93.3**	**46.7**	**23.3**	**2**	**0.046**
MWCNT Cost *Disposal of PPE Cost	**89.1**	**44.6**	**23.3**	**1.91**	**0.057**
MWCNT Cost* Cycle Time	**54**	**27**	**23.2**	**1.16**	**0.246**
Energy Cost* Disposal of PPE Cost	**91.9**	**46**	**23.3**	**1.98**	**0.05**
Energy Cost *Cycle Time	**2983.9**	**1492**	**23.2**	**64.23**	**0**
Disposal of PPE Cost *Cycle Time	**52.5**	**26.2**	**23.2**	**1.13**	**0.26**
Process Yield* MWCNT Cost* Energy Cost	**-32.1**	**-16.1**	**29.1**	**-0.55**	**0.581**
Process Yield *MWCNT Cost* Disposal of PPE Cost	**-31.4**	**-15.7**	**29.1**	**-0.54**	**0.59**
Process Yield *MWCNT Cost *Cycle Time	**-17.2**	**-8.6**	**28.7**	**-0.3**	**0.765**
Process Yield* Energy Cost* Disposal of PPE Cost	**-29.1**	**-14.5**	**29.1**	**-0.5**	**0.618**
Process Yield *Energy Cost *Cycle Time	**-362.4**	**-181.2**	**28.7**	**-6.31**	**0**
Process Yield* Disposal of PPE Cycle* Time Cost	**-20**	**-10**	**28.7**	**-0.35**	**0.729**
MWCNT Cost *Energy Cost *Disposal of PPE Cost	**132.9**	**66.4**	**28.6**	**2.33**	**0.021**
MWCNT Cost* Energy Cost *Cycle Time	**83.8**	**41.9**	**28.5**	**1.47**	**0.143**
MWCNT Cost* Disposal of PPE Cost* Cycle Time	**78.1**	**39.1**	**28.5**	**1.37**	**0.172**
Energy Cost* Disposal of PPE Cost* Cycle Time	**78.9**	**39.4**	**28.5**	**1.39**	**0.167**
Process Yield* MWCNT Cost* Energy Cost* Disposal of PPE Cost	**-47.7**	**-23.9**	**36**	**-0.66**	**0.509**
Process Yield* MWCNT Cost* Energy Cost* Cycle Time	**-23**	**-11.5**	**35.4**	**-0.32**	**0.746**
Process Yield* MWCNT Cost* Disposal of PPE Cost* Cycle Time	**-22.2**	**-11.1**	**35.4**	**-0.31**	**0.754**
Process Yield* Energy Cost* Disposal of PPE Cost* Cycle Time	**-29.3**	**-14.7**	**35.4**	**-0.41**	**0.679**
MWCNT Cost* Energy Cost* Disposal of PPE Cost* Cycle Time	**120.2**	**60.1**	**34.9**	**1.72**	**0.087**
Process Yield* MWCNT Cost* Energy Cost* Disposal of PPE Cost* Cycle Time	**-37.2**	**-18.6**	**43.7**	**-0.43**	**0.671**

The P-value for the main effects and the two, and three-way interactions indicates that they are significant as shown on the analysis of variance table (Table 3-10). However, the P-value is 0.615 and 0.617 for the four and five-way interactions respectively which indicates that its effect on the total cost is not significant because is higher than 0.05.

Table 3-10 Analysis of variance for total cost of satellite batteries (high EHS)

Source	DF	SS	MS	F	P
Main Effects	5	5909994923	1181998985	20355.16	0.000
2- way interactions	10	287351886	28735189	494.85	0.000
3- way interactions	10	2873962	287396	4.95	0.000
4-way interactions	5	206565	41313	0.71	0.615
5-way interactions	1	10540	10540	0.18	0.671

As shown in Figure 3-24, the normal plot of the standardized effects shows the main effects have a higher impact on the total cost than the interaction effects as they are further from the fitted line. The interaction effects are centered around zero. The process yield, MWCNT cost, energy cost, and cycle time at forming step are identified as significant main effects. From the two-way interaction effects, the interactions between (1) process yield and MWCNT cost, (2) process yield and energy cost, (3) process yield and cycle time, (4) MWCNT cost and energy cost (5) energy cost and cycle time are significant. From the three-way interaction effects, the interactions among (1) process yield, energy cost, and cycle time (2) MWCNT cost, energy cost, and disposal PPE hazardous waste are significant.

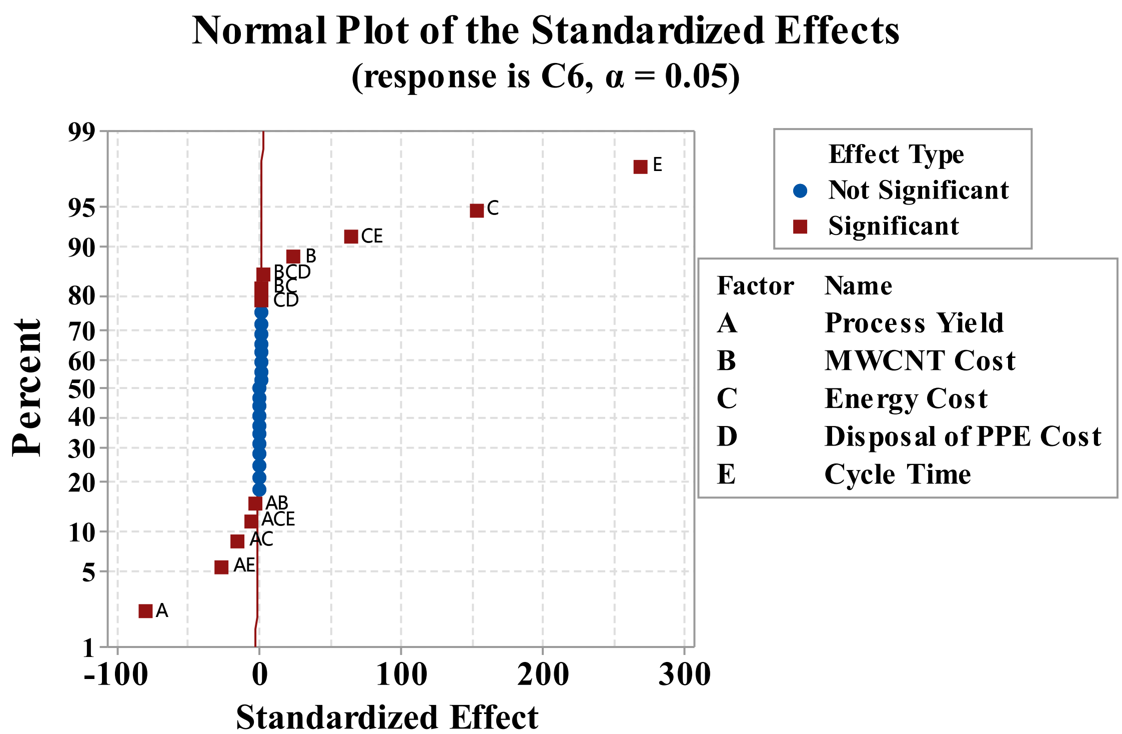


Figure 3-24 Normal plot of the standardized effects for satellite batteries –High EHS

Main and interaction effects on manufacturing unit cost of battery for computers are shown in Figure 3-25 and Figure 3-26. Similar to the satellite batteries, both energy and cycle time have significant effect on manufacturing unit cost of battery with CNTs for portable computers. Cost of MWCNTs has less effect on manufacturing unit cost in computer batteries due to the low amount of MWCNT in the computer batteries compared with satellite batteries. Cost of disposal of PPE hazardous waste has the least effect on total manufacturing unit cost as compared to other parameters. Similar to the previous case, process yield has negative effect on manufacturing unit cost. However, it has more effect on the manufacturing unit cost of battery for computers because variable cost has more effect on manufacturing unit cost of battery for computers.

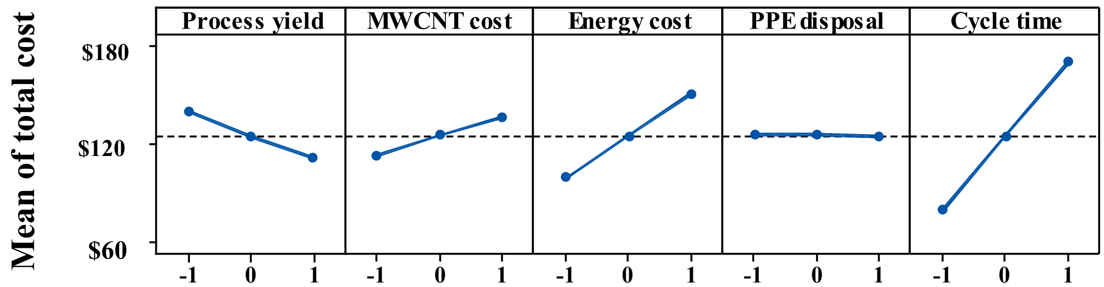


Figure 3-25 Main effects plot diagram for computer batteries for high EHS scenario at the mid-value level (0)

Figure 3-26 shows the effect of the factor pairs on manufacturing unit cost for computer batteries. The interaction between the factors, energy cost and cycle time, has higher effects on the manufacturing unit cost of batteries for computers whereas the interaction between the cost of disposal of PPE hazardous waste and cycle time at forming step has the least effect on total manufacturing unit cost. Figure 3-13 also indicates when the energy cost and cycle time are increased, the manufacturing unit cost increases significantly.

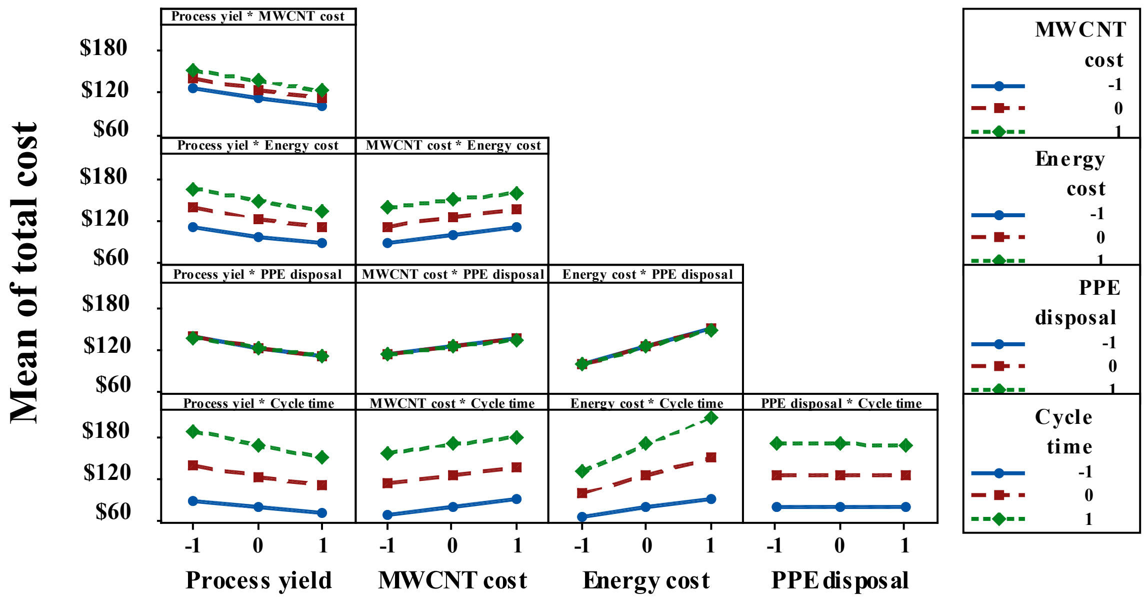


Figure 3-26 Interaction plot diagram for computer batteries for the high EHS scenario

Response surface graph (Figure 3-27) shows the effect of the energy cost and cycle time on manufacturing unit cost of batteries for computers. Similar to in manufacturing satellite batteries, both cycle time at forming step and energy cost are the factors that have the main effect on manufacturing unit cost of computer batteries. Although, energy cost has less effect on total unit cost of computers compared with the effect of cycle time at forming step, to minimize the manufacturing unit cost and promote sustainable manufacturing, both cycle time at forming step and type of energy used during battery manufacturing should be optimized. Therefore, investing on better technologies for producing the batteries and using low cost energy is recommended.

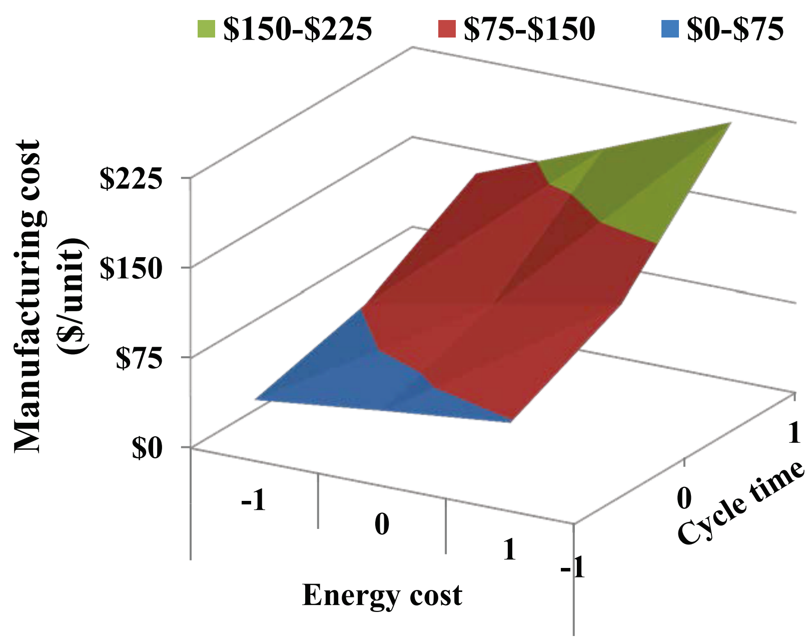


Figure 3-27 Surface graph for computer MWCNT-enabled batteries for parameters with greatest influence on manufacturing cost, holding all other parameters at base level (0) values (for high EHS scenario)

The main factors which have the highest impact on the total unit cost (computer battery) were shown in Figure 3-25. The next step is to generate the standardized effect plot by developing a two-level design with five factors for computer batteries. Table 3-11 shows all the possible combinations. As previously mentioned, the values in the P column of Table 3-11 are used to determine which of the effects are significant. Also, the blue highlighted factors in Table 3-11 and Table 3-12 are identified as significant since they have P-values less than 0.05. The T value for the cycle time is higher with a value of 304.99 than the rest of the main effects, meaning that its impact is highest on the total cost.

Table 3-11 Estimated effects and coefficients for computer batteries (high EHS)

Term	Effect	Coefficient	SE Coeff	T	P
Constant		173.978	0.205	849.2	0
Process Yield	-40.003	-20.001	0.253	-79	0
MWCNT Cost	4.118	2.059	0.251	8.2	0
Energy Cost	87.269	43.634	0.251	173.76	0
Disposal of PPE Cost	0.902	0.451	0.251	1.8	0.074
Cycle Time	152.975	76.488	0.251	304.99	0
Process Yield*MWCNT Cost	-0.605	-0.302	0.312	-0.97	0.333
Process Yield *Energy Cost	-10.478	-5.239	0.312	-16.81	0
Process Yield* Disposal of PPE Cost	-0.277	-0.138	0.312	-0.44	0.658
Process Yield *Cycle Time	-18.288	-9.144	0.309	-29.58	0
MWCNT Cost *Energy Cost	1.257	0.628	0.308	2.04	0.043
MWCNT Cost *Disposal of PPE Cost	1.229	0.615	0.308	2	0.047
MWCNT Cost* Cycle Time	0.781	0.39	0.307	1.27	0.205
Energy Cost* Disposal of PPE Cost	1.259	0.629	0.308	2.04	0.042
Energy Cost *Cycle Time	44.796	22.398	0.307	72.88	0
Disposal of PPE Cost *Cycle Time	0.75	0.375	0.307	1.22	0.224
Process Yield* MWCNT Cost* Energy Cost	-0.328	-0.164	0.385	-0.43	0.671
Process Yield *MWCNT Cost* Disposal of PPE Cost	-0.337	-0.168	0.385	-0.44	0.662
Process Yield *MWCNT Cost *Cycle Time	-0.243	-0.121	0.38	-0.32	0.75
Process Yield* Energy Cost* Disposal of PPE Cost	-0.372	-0.186	0.385	-0.48	0.629
Process Yield *Energy Cost *Cycle Time	-5.542	-2.771	0.38	-7.29	0
Process Yield* Disposal of PPE Cycle* Time Cost	-0.298	-0.149	0.38	-0.39	0.696
MWCNT Cost *Energy Cost *Disposal of PPE Cost	1.893	0.946	0.378	2.5	0.013
MWCNT Cost* Energy Cost *Cycle Time	1.084	0.542	0.377	1.44	0.152
MWCNT Cost* Disposal of PPE Cost* Cycle Time	1.138	0.569	0.377	1.51	0.132
Energy Cost* Disposal of PPE Cost* Cycle Time	1.095	0.547	0.377	1.45	0.148
Process Yield* MWCNT Cost* Energy Cost* Disposal of PPE Cost	-0.662	-0.331	0.477	-0.69	0.489
Process Yield* MWCNT Cost* Energy Cost* Cycle Time	-0.33	-0.165	0.468	-0.35	0.725
Process Yield* MWCNT Cost* Disposal of PPE Cost* Cycle Time	-0.4	-0.2	0.468	-0.43	0.67
Process Yield* Energy Cost* Disposal of PPE Cost* Cycle Time	-0.338	-0.169	0.468	-0.36	0.718
MWCNT Cost* Energy Cost* Disposal of PPE Cost* Cycle Time	1.602	0.801	0.462	1.73	0.084
Process Yeild* MWCNT Cost* Energy Cost* Disposal of PPE Cost* Cycle Time	-0.607	-18.6	43.7	-0.43	0.671

Table 3-12 shows the P-value for the main effects, two, three, four, and five-way interactions of the factors and determines the significant ones. As shown in Table 3-12, the P-value of the main effects, two, and three-way interactions is 0 which indicates its effect on the total cost is significant because the p-value is higher than 0.05 unlike the four and five-way factor interactions.

Table 3-12 Analysis of variance for total cost of computer batteries (high EHS)

Source	DF	SS	MS	F	P
Main Effects	5	1303396	260679	25642.99	0.000
2- way interactions	10	64751	6475	636.96	0.000
3- way interactions	10	648	65	6.38	0.000
4-way interactions	5	37	7	0.74	0.597
5-way interactions	1	3	3	0.28	0.600

Normal plot of the standardized effects is shown in Figure 3-28. The graph indicates the main effects have a higher impact on the total cost than the interaction effects because of being further from the fitted line. Similar to satellite batteries, the process yield, MWCNT cost, energy cost, and cycle time at forming step are identified as significant main effects on total unit cost in computer battery manufacturing. From the two-way interaction effects, the interactions between (1) Process Yield *Energy Cost (2) Process Yield *Cycle Time (3) MWCNT Cost *Energy Cost (4) MWCNT Cost *Disposal of PPE Cost (5) Energy Cost* Disposal of PPE Cost (6) Energy Cost *Cycle Time are significant. From the three-way interaction effects, the interactions among (1) process yield, energy cost, and cycle time (2) MWCNT cost, energy cost, and disposal PPE hazardous waste are significant.

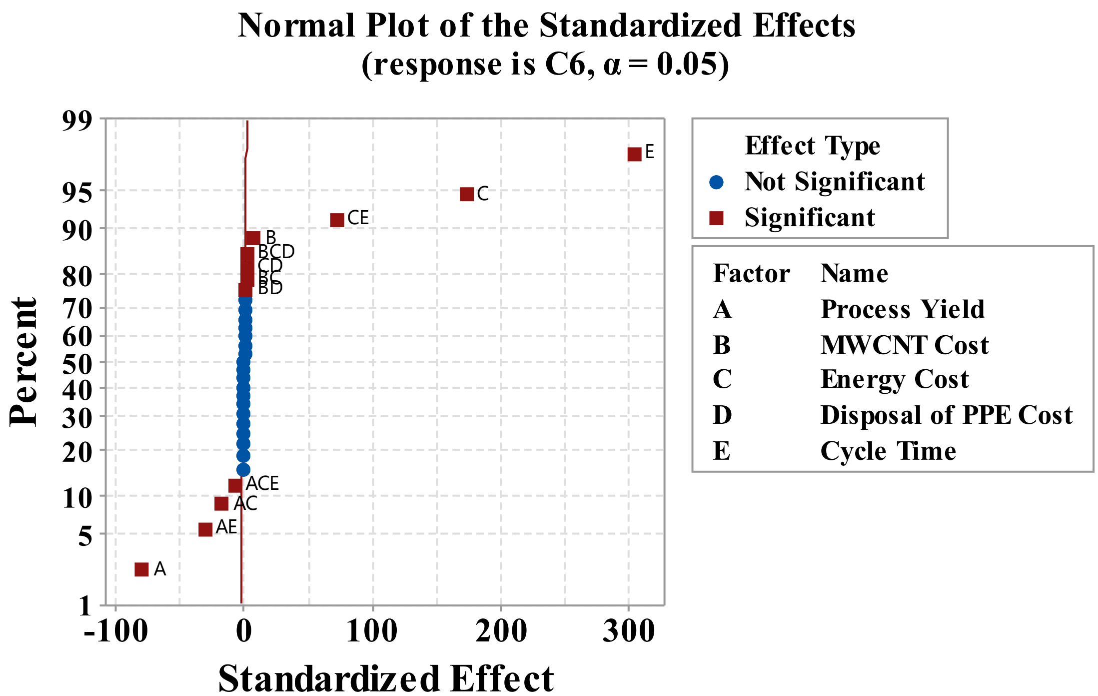


Figure 3-28 Normal plot of the standardized effects for satellite batteries –High EHS

3.8. Conclusion

Given the manufacturing process assumptions and investigating the PBCM results, the dominant cost driver parameters toward the manufacturing unit cost of CNT NMC batteries are verified. Energy cost and cycle time have the most effect on manufacturing unit cost for satellite and computer batteries, respectively. With the increase in MWCNTs use in satellite batteries and the mass of other materials, the manufacturing unit cost increases significantly. Cycle time at forming step has significant effect on manufacturing unit cost for both satellite and computer batteries. As cycle time for forming step increases, the manufacturing cost increases significantly due to the increase in the energy consumption at forming step. Energy cost has also major effect on manufacturing unit cost of lithium-ion batteries with CNTs. Since energy cost is one of the cost drive parameter at forming step, it influences the cost at forming step. By developing the economic assessment methodology and its design of experiment analysis, the best scenario in terms of alternative materials, resources, number of labors, and number of production lines can be determined.

CHAPTER 4 ENVIRONMENTAL ASSESSMENT METHODOLOGY

In this Chapter, the manufacture of carbon-nanotube-enhanced lithium-ion batteries (MWCNT NMC batteries) in portable computers is investigated from an environmental perspective and compared with conventional NMC batteries. An environmental analysis of process changes considers non-renewable energy, renewable energy, and the combination of both types of energy during the manufacturing of batteries.

Data for life cycle assessment of traditional NMC batteries and of MWCNT NMC batteries in computers are gathered, either from literature, industry from experts, or modeling tools. More detailed objectives for each step are defined in the sections.

4.1. Life Cycle Assessment

In recent years, environmental sustainability has been one of the critical topics considered during the products' life cycle (Compact 2009). An appropriate environmental analysis methodology must investigate all environmental impacts of a system. To fulfill these requirements, life cycle assessment (LCA) methodology was developed. LCA is a tool for assessing, investigating, and determining the potential environmental impacts from any manufacturing processes, products, and services over their lifetime (Agency 1993, Agency 2006, Standardization 2006). LCA was first applied in 1969 by a beverage-company concerning product-packaging (Baumann and Tillman 2004). Application of LCA methodology over the product life including mining and refining, distribution, manufacture, use, and disposal identifies the overall environmental impacts. Figure 4-1 explains the life cycle stages and the corresponding inputs and outputs for an LCA study.

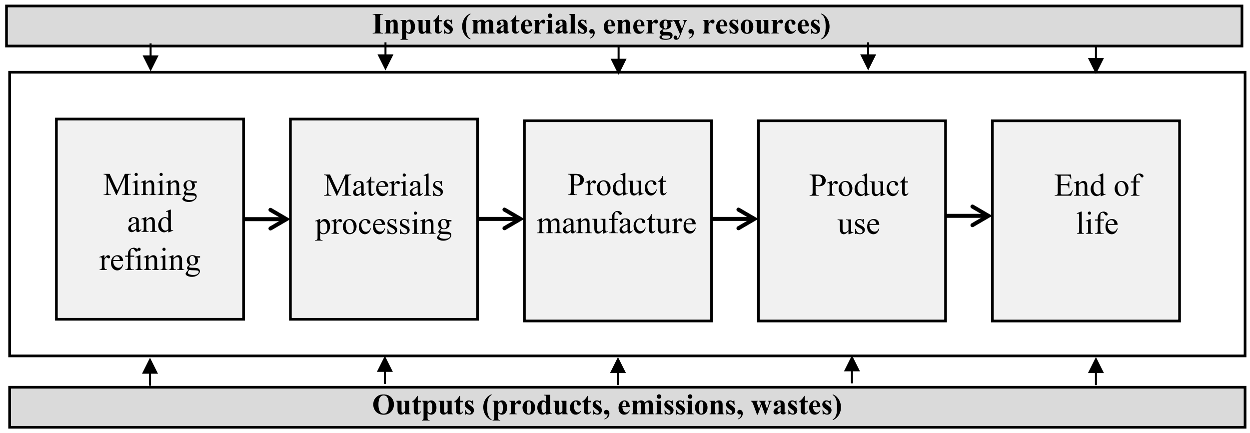


Figure 4-1 Life cycle stages (Amarakoon 2013)

The International Standards Organization (ISO), a non-governmental organization which sets and specifies all of the commercial and international industrial standards, describes the LCA phases and stages in detail. The ISO 14040 series illustrates LCA standards and guidelines. The ISO 14040-14044 guidelines emphasizes that there are four independent major phases to an LCS study (Standardization 2006, Amarakoon 2013):

1. Goal and scope definition (ISO 14044)
2. Inventory analysis (Life cycle inventory, LCI) (ISO 14044)
3. Impact assessment (Life cycle impact assessment, LCIA) (ISO 14044)
4. Interpretation of results (ISO 14044)

LCA can also be used for product design and development, marketing, strategic planning and other company decisions and more importantly public policy making as a basis of the law (Organization 2006, Standardization 2006).

Figure 4-2 illustrates the systematic and dynamic elements. Each of the four phases is described in more detail.

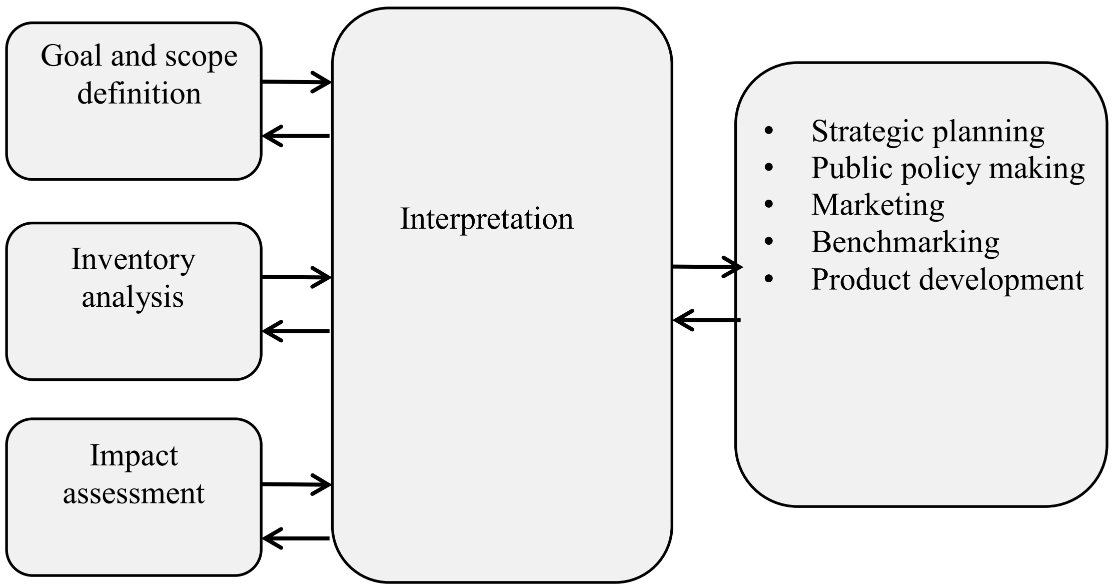


Figure 4-2 Life cycle assessment methodology (Standardization 2006)

4.1.1. Goal and scope definition

In the first stage of the LCA, the goal of the project describes the purpose and intention of carrying out the study, and the scope defines the boundary desired to achieve the goal. The first phase of LCA methodology is a very critical step because the study direction is illustrated. The boundaries - the stages of the life cycle included- determine which resources are included. Some of the parameters that are identified in the goal and scope definition phase include system boundaries, functional unit, data organization, environmental parameters, and evaluation method (Agency 2006, Standardization 2006, Amarakoon 2013).

The final results of LCA study are varied and are influenced significantly by the decisions and the selected parameters during the goal and scope definition phase. For instance, considering system boundaries, there are three common LCA system boundaries including cradle-to-gate, cradle-to-grave, and cradle-to-cradle. During the cradle-to-gate analysis, the environmental footprint of all inputs and outputs from raw material acquisitions (cradle) to the factory gate are analyzed while the environmental footprint of all inputs and outputs from raw material acquisitions to use and disposal stage are analyzed during cradle-to-grave system boundaries (Agency 2006).

Another important LCA parameter is the functional unit, which provides a basis for comparison for two or more alternatives. Based on the functional unit, the environmental footprints are analyzed and compared with the same function of the similar products (Agency 1993, Agency 2006).

4.1.2. Inventory analysis

To determine, measure, and quantify the raw material requirements, energy requirement, equipment used, atmospheric emissions, waterborne emissions, and solid wastes of the entire life cycle of the products, inventory analysis is undertaken (Agency 2006, Standardization 2006).

Depending on the goal and the scope of the LCA study, inventory collection differs and often is very time-consuming. LCI data could be gathered from different sources such as:

industry data reports, laboratory reports, inventory databases, and direct measurement. Based on the functional unit of a product, data for the input and output materials for each stage in the life cycle are collected for analysis (Agency 2006).

4.1.3. Impact assessment

In the third phase of the life cycle assessment methodology, the potential human health and the environmental impacts for the inventory are identified and evaluated. LCIA consists of two significant steps that include classification and characterization. The inventory results are classified based on their effect on the environment. First, the desired environmental impact categories are identified, and then the relevant substances are categorized into the selected impact categories (Agency 2006).

During the classification step, all collected data during LCI is grouped and assigned to desired impact categories. For instance CO_2 emission is assigned to the global warming potential (GWP) impact category. Details are presented elsewhere (Baumann and Tillman 2004). In the characterization step, the assigned data are used to calculate impact categories (Standardization 2006). The results are shown in a mass-equivalent mode e.g., GWP is mostly displayed in kilogram CO_2-equivalents (Frischknecht, Jungbluth et al. 2007).

Impact assessment characterizes the environmental impacts and evaluates the contributions of each impact category most readily through the use of software packages such as SimaPro™ software (Standardization 2006, Consultants 2011). The software entitle “System for Integrated Environmental Assessment of Products” (SimaPro™) is a professional LCA tool that facilitates evaluation of the environmental performance of the products (Consultants 2011). SimaPro^{TM} includes the several inventory databases along with the different impact assessment methods, which vary for different regions. In this study, the Ecoinvent 2.2 inventory database and the TRACI 2 impact assessment method are used (Bo Weidema 2010).

Ecoinvent database is one of the most comprehensive and recognized international LCI databases. It includes thousands of industrial processes and LCI datasets in different areas such as transport, energy supply, packaging, and chemicals.

The Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI 2) is a LCIA method that was developed in the USA (Frischknecht, Jungbluth et al. 2007). TRACI 2 calculates equivalent masses for the environmental impact categories e.g., global warming, acidification, eutrophication, ozone depletion, and human health (Frischknecht, Jungbluth et al. 2007). In TRACI 2, the human health category is divided into three subcategories: carcinogenic, non-carcinogenic and respiratory (Frischknecht, Jungbluth et al. 2007) .

Several impact assessment indicators are used to assess the environmental impacts of MWCNT NMC batteries, with the leading indicator assumed as the cumulative energy demand (CED). CED indicator emphasizes the energy consumption throughout the life cycle (Frischknecht, Jungbluth et al. 2007). Energy can be tracked as renewable or non-renewable sources. In this study the environmental impact assessment of MWCNT NMC batteries manufacturing is investigated by considering using non-renewable, renewable and the combination of both renewable and non-renewable energy during the manufacturing.

4.1.4. Interpretation

The final phase of LCA study is the interpretation, which includes analysis of the major environmental impacts of the product and sensitivity analysis. To make a complete, detailed, feasible, and reliable recommendation, the inventory analysis and the environmental impact assessment results for the defined study goal are investigated closely. From this information and the results, the LCA findings can be comprehensive, understandable, and informative for the decision makers (Agency 2006, Standardization 2006).

4.2. Literature Review of Life Cycle Assessment of Batteries

Steele and Allen (1998) used the LCA techniques to analyze and compare the potential health and the environmental impact associated with recycling and waste management of four different battery technologies including: lead-acid, nickel-cadmium, nickel-metal hydride, and sodium-sulfur. In terms of the environmental impact, they concluded that recycling of lead-acid and nickel-cadmium batteries had greater impact and raised more concern compared with the recycling of nickel-metal hydride and sodium-sulfur batteries. With respect to disposal, there were more uncertainties and concerns related to the nickel-metal hydride and the sodium-sulfur batteries compared with the other two batteries. They also showed that during the recycling processes, the sodium-sulfur and the nickel-metal hydride batteries posed a lower rated level of exposure compared with the lead-acid and the nickel-cadmium batteries. With respect to disposal, lead-acid batteries were the least desirable. Overall in all four categories, the nickel-metal hydride batteries were the most favored ones from recycling aspect and the nickel-cadmium batteries were the preferred ones from the disposal aspect.

Rydh and Karlstrom (2002) used the LCA approach to evaluate the environmental impacts of recycling the nickel-cadmium (NiCd) batteries. The results indicated that in battery manufacturing, the primary energy and the CO_2 emission were the significant parameters that needed to be monitored. They showed that 55% of the CO_2 emission was produced from the battery manufacturing, 44% from the raw materials production, and 0.8% from the battery distribution. The batteries manufactured from the virgin cadmium and nickel had 16% greater primary energy compared with the ones manufactured from the recycled metals. From an environmental standpoint, the optimum recycling rate of NiCd batteries was close to 100%.

The estimation and comparison of greenhouse gas (GHG) emissions from plug-in-hybrid vehicles (PHEVs), conventional gasoline vehicles (CVs), and hybrid-electric cars (HEVs) was performed by considering three approaches by Samaras et al (2008). They concluded that the GHG emission reductions in PHEVs were highly dependent on the energy sources of the electricity production. During the use phase under the US average GHG intensity of electricity, GHG emissions in PHEVs were reduced by 38-41% compared with CVs and 7-12% compared with HEVs. Under the low-carbon electricity generation, GHG emissions in PHEVs decreased by 51-63% and 30-47% compared with CVs and HEVs, respectively.

Zackrisson and Avellan (2010) applied the LCA methodology to optimize the design of the lithium-ion batteries for the plug-in hybrid electric vehicles. Lithium-ion batteries with two different solvents were considered. Five different environmental impact categories that were tracked during the production, use phase, and EOL of batteries including: global warming, acidification, ozone depletion, photochemical smog, and eutrophication. They showed from the environmental standpoint, that the production phase of the lithium-ion battery had greater environmental impact compared with the other phases of its life cycle. The production phase dominated in four environmental impact categories.

Notter et al. (2010) studied the use of the lithium-ion batteries and their environmental impacts in electric cars by using the LCA methodology. The environmental and human health impacts were assessed through four different impact assessment categories: abiotic depletion potential, nonrenewable cumulated energy demand, global warming potential, using Ecoindicator99 H/A. Ecoindicator99 H/A is concerned more with the toxicity to humans and the ecosystem, while the other impact evaluation methods are driven exclusively by the use of the minerals and energy. The resulting environmental impacts of the use phase of the lithium-ion batteries were relatively small compared with the environmental impact during the production phase of life cycle of the batteries. Ecoindicator99 H/A showed the production of the anodes (graphite and copper) produced the highest environmental impacts, while other evaluation methods indicated the production of the cathodes (aluminum+$LiMn_2O_4$) generated greater environmental impact.

Stamp et al. (2012) used the LCA methodology to investigate how the changes in the environment on different resource provisions would affect the impact on the product and service level. They considered three different supply options for the lithium carbonate: brine, ore, and seawater, and compared results from three impact assessment methods: cumulative energy demand, Ecoindicator99, and the global warming potential. The result showed that lithium-ion batteries with lithium obtained from the seawater process had lower environmental impact compared with the other two processes recovering lithium under the different impact assessment methods. Also, they showed that the environmental impact of the lithium-ion batteries that obtained the lithium from all three different scenarios in electric cars had between 10 and 45% lower impact compared with the internal combustion engine vehicles.

Frischknecht and Flury (2011) investigated the life cycle-based climate change impact of the manufacturing phase of 1 kg lithium-ion batteries with different life cycle inventories. Different data inventories used were: Ecoinevent data v2.2 (Bo Weidema 2010), ESU-services (2010) and Zackrisson et al. (2010). The results for the climate change impacts of manufacturing of 1 kg lithium-ion batteries from different data bases were: 5.8 kg CO_2/km, 17.1 kg CO_2/km and 15.5-25.5 kg CO_2/km for Ecoinevent data v2.2, ESU-services and Zackrisson databases, respectively. The results of LCA studies of the electric cars that were collected from different LCI data sets were compared with the conventional gasoline vehicles.

LCA of three batteries (nickel metal hydride, nickel cobalt manganese lithium-ion, and iron phosphate lithium-ion) for plug-in hybrid and the electric vehicles were investigated and their environmental impacts have been analyzed by Bettz et al (2011). The environmental impact results showed that the nickel metal hydride battery performed significantly worse than the other two batteries except for the ozone depletion potential. Also, the results specified that the overall global warming impacts were 35 g CO_2-eq/km for the nickel metal hydride battery, 19 g CO_2-eq / km for the nickel cobalt manganese lithium-ion battery, and 14 g CO_2-eq/km for the iron phosphate lithium-ion battery.

Several studies evaluated the environmental assessment of five different rechargeable batteries, lead-acid (PbA), nickel‑cadmium (NiCd), nickel-metal hydride (NiMH), sodium-sulfur (Na/S), and lithium-ion (Li-ion) batteries, by applying LCA methodology. Various emissions such as, CO, NO_x, SO_x, CH_4, N_2O, and CO_2 to air, water, and solid were collected and assessed for the production and recycling phase of the batteries. The emissions to air and water during the life cycle of 1 kg of the each battery were calculated.

4.3. MWCNT NMC Batteries Assessment Boundaries

The MWCNT lithium-ion cell specifications described in Chapter 3 (Table 3-6) for portable computers are environmentally assessed. This battery has an anode made of graphite with a cathode made of MWCNTs and NMC materials. The unit by which it is evaluated in this study (functional unit) is considered to be one MWCNT NMC battery to power a portable computer. The inventory materials and the environmental impacts are shown in terms of weight of a battery in kg. Total weight of the battery is assumed to be 0.41 kg while the energy density of each battery cell is 228 Wh/kg.

The life-cycle stages and the corresponding input and output materials in a LCA study is shown in Figure 4-1. The environmental impacts of each of life-cycle stages are assessed for cradle-to-gate. This study focuses only on the raw materials and the manufacturing of a battery product. During LCI phase, raw materials, energy, equipment used, and solid wastes are gathered. Before collecting all the input resources, the detailed process flow diagram for the manufacture of MWCNT NMC batteries should be developed. The process flow diagram includes all life-cycle-stages of the MWCNT NMC batteries. The extraction and materials needed for the manufacturing of NMC batteries is shown in the upstream stages. The anode, cathode, separator, electrolyte, and other materials for different battery components as well as upstream materials processing for the MWCNT cathode are included in the detailed process flow diagram which is shown in Figure 4-3.

Converting and translating the environmental burdens which are recognized in the LCI phase into environmental impacts occurs during LCIA study. Quantitative results of the environmental impacts of the manufacturing of MWCNT NMC batteries as well as their impacts on the human health are identified during the third phase of LCA study. In this study the Ecoinvent™ inventory database (one of the inventory databases available in SimaPro™) and TRACI 2 impact assessment method are employed. The different impact categories are evaluated for MNCNT CNT battery product and the corresponding indicators are shown in the following.

- Global warming (kg CO2 eq)
- Acidification (H+ moles eq)
- Carcinogenics (kg benzene eq)

- Non carcinogenics (kg toluene eq)
- Respiratory effects (kg PM2.5 eq)
- Eutrophication (kg N eq)
- Ozone depletion (kg CFC-11 eq)
- Ecotoxicity (kg 2,4-D eq)
- Smog (g NOx eq)

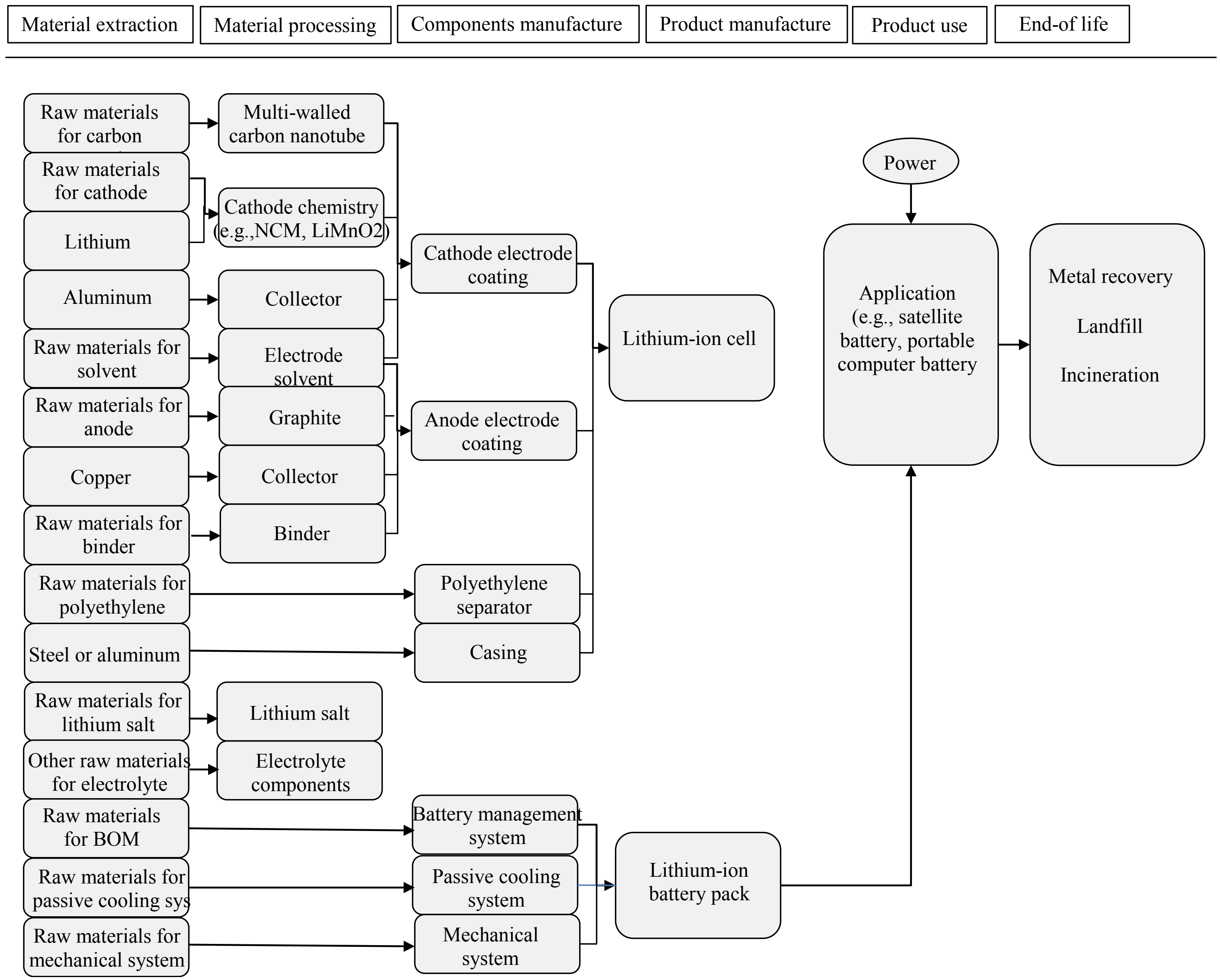


Figure 4-3 Proposed process Flow Diagram for the Manufacture of MWCNT NMC Batteries for Computer battery (Amarakoon 2013)

4.3.1. Life Cycle Inventory of MWCNT NMC Batteries

To construct a LCI for the MWCNT NMC battery, the manufacturing processes, model inputs, including physical parameters and assumptions must be defined. LCI of a product system consists of a set of inventories for processes throughout the life cycle of the product – from upstream materials extraction, materials processing, product manufacture, product use, and end-of-life which was shown in Figure 4-3. The inventory of input and output flows for each process is presented in Figure 4-4. The values are generated using parameters from PBCM developed and discussed in Chapter 3.

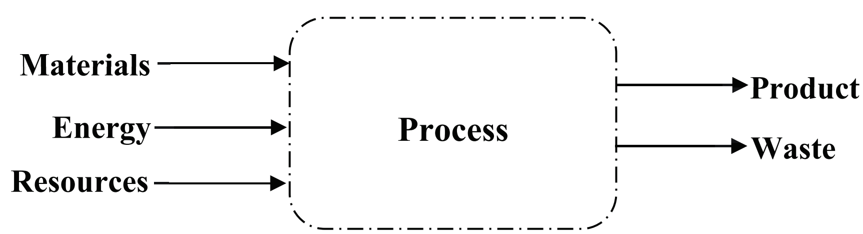


Figure 4-4 Process Input and Output Flows (Amarakoon 2013)

The results on the life cycle inventory of MWCNT NMC battery fabrication are presented. The data collection method, data resources, and inventory methodology is explained. Then, the fabrication steps are described in detail based upon unit run operations. The energy and input materials required to carry out the process step is adjusted based on the unit run operations. Similarly, the amount and types of output materials (emissions, gas) are calculated for all steps using an annual production volume of 1,000,000 computer batteries.

4.3.2. Methodology and Data Sources

In this section, the descriptions and details of the LCI data categories and data sources for each process step of MWCNT NMC batteries manufacturing are discussed. The manufacturing data e.g., the amount of raw materials, energy, and resources were collected from the lithium-ion battery manufacturing company located in East Greenwich, Rhode Island. This includes documenting the types of input materials, exploring waste treatment of used materials, monitoring equipment used, and estimating energy consumption in manufacturing of lithium-ion batteries containing no CNTs. Additionally, we used some scientific literature, laboratory reports, and LCI data available in the Ecoinvent (one of the SimaPro databases) LCA software tool (Notter, Gauch et al. 2010, Zackrisson, Avellán et al. 2010, Majeau-Bettez, Hawkins et al. 2011, Shanika Amarakoon 2013, Ates, Mukerjee et al. 2014, Shah, Ates et al. 2014). Upstream materials and corresponding components and data sources are shown in Table 4-1.

Table 4-1 Upstream material data resources

Battery component	Material name	Data sources
Anode	Graphite	Ecoinvent and (Notter, Gauch et al. 2010)
	Copper foil	Ecoinvent
Cathode	Lithium-nickel cobalt manganese oxide (Li-NCM battery)	(Majeau-Bettez, Hawkins et al. 2011)and Ecoinvent
Cathode and anode	Binder	Ecoinvent
	Solvent	Ecoinvent
Secretor	Polyolefin	Ecoinvent
Casing	Polypropylene resin	Ecoinvent
Electrolyte	Lithium hexaflourophosphate (LiPF6)	Ecoinvent and (Notter, Gauch et al. 2010)
BMS	Copper wiring	Ecoinvent
	Steel	Ecoinvent
Passive cooling system	Steel	Ecoinvent
	Aluminum	Ecoinvent

In addition to the materials in Table 4-1, the environmental impacts of MWCNTs were separately assessed. An inventory for MWCNTs based on the study from Shah et al. (2014) and other sources (de las Casas and Li 2012, Ko, Lee et al. 2012, Vinayan, Nagar et al. 2012, Amarakoon 2013). The MWCNT inventory data was included in the product system to calculate its environmental impacts. Next, the bill of materials for manufacturing of NMC batteries for portable computers is presented in Table 4-2.

Table 4-2 Components of MWCNT NMC batteries for computers (battery weighing 0.41 kg) (Amarakoon 2013)

Battery component	Mass percentages (%)
Cathode	**30%**
NMC material	21%
Aluminum (collector)	5%
Carbon black	1 %
MWCNT	0.93%
PVDF	2%
Other materials	0.9%
Anode	**25%**
Graphite	16%
Copper (collector)	8%
Carbon black	1%
Other materials	0.3%
Separator	**4%**
Polyethylene	4%
Electrolyte	**10%**
Organic carbonate and lithium salt	10%
Cell container	**1%**
Can/case (aluminum)	1%
Module container	**5%**
Case (aluminum)	5%
Pack container and BMS	**25%**
Steel	13%
Passive cooling system	10%
Copper wiring	1%
Printed wire board	1%
Total	**100%**

As shown in Table 4-2, the weight for each component of batteries for portable computers considering total weight of 0.41 kg per battery is presented. The detailed manufacturing process steps of MWCNT NMC batteries were shown in Figure 4-5. Based on the manufacturing processes of MWCT NMC batteries and bill of materials for the each battery chemistry (Table 4-2), MWCNT NMC batteries for portable computers are manufactured. The energy consumption and cycle time of each manufacturing process step are presented in section 4.3.3.

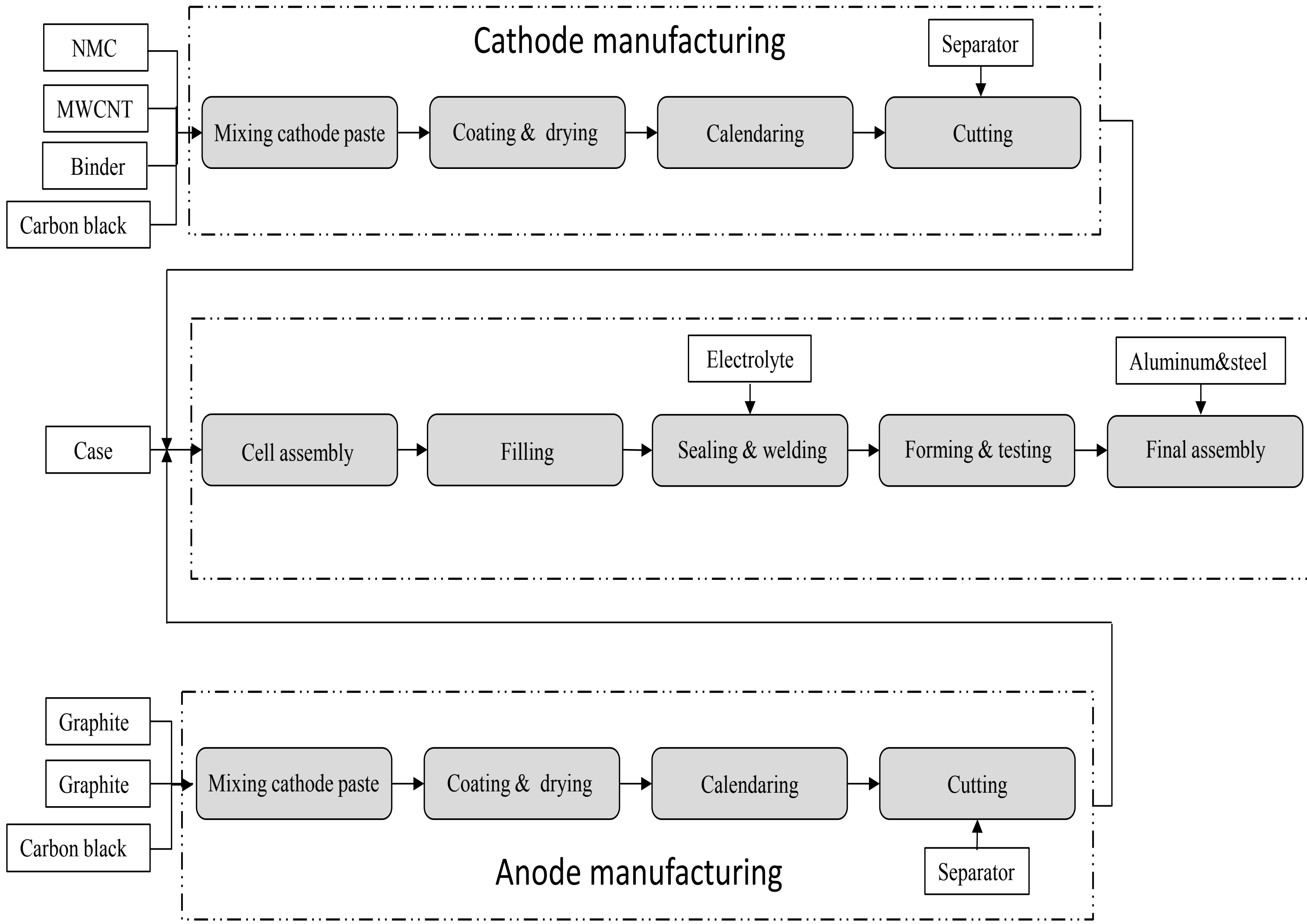


Figure 4-5 Proposed detailed manufacturing processes of MWCNT NMC batteries (Amarakoon 2013)

4.3.3. Inventory Structure and Fabrication Steps

To develop life cycle inventory data of MWCNT NMC batteries, all inputs, resources and utility data were collected per mass (kg) basis. The battery is built based on its components mass percentages (bill of material) and the energy capacity (kWh/charge cycle) of the battery. All data were converted to a per battery basis, using information about specific energy (kWh/kg) and the mass of one battery (kg). The total weight of the computer battery, its cell energy density, and the battery life are shown in Table 4-3. Note that a functional unit of one battery does not account for the differences in energy density or life time. Comparison of the attributes is discussed later.

Table 4-3 Specifications for the basis comparison of two computer battery systems

Battery Specification	MWCNT NMC Battery	Conventional NMC Battery
Cell energy density (Wh/kg)	228 Wh/kg	193 Wh/kg
Total battery weight (kg)	0.41 kg	0.41 kg
Battery life	6 yrs	3 yrs

The first manufacturing step of MWCNT NMC batteries is cathode and anode mixing. The energy use and material inputs/outputs for Step 1 is summarized in Table 4-4. The composition and the production of the anode was found from (Notter, Gauch et al. 2010, Amarakoon 2013) and Ecoinvent2.2 database while, cathode composition was found in (Notter, Gauch et al. 2010, Majeau-Bettez, Hawkins et al. 2011, Inc 2014, Shah, Ates et al. 2014). The ratio of all the input materials as well as the current collectors for anode and cathode was modified based on Table 4-2.

Table 4-4 Step 1 – Materials inventory & energy use

Cathode & Anode Mixing	
Total cycle time/cell	0.0002 hr
Energy	**[kWh/cell]**
Total energy /cell	0.0068 kwh
Material	**[kg/cell]**
<u>Input</u>	
Cathode active material (NMC)	0.014
Anode active material(Graphite)	0.011
NMP	0.009
PVDF	0.001
MWCNT	0.001
Carbon black	0.0017
Deionized water	0.004
Sodium hydroxide	0.00033
Sulphuric acid	0.00022
<u>Output</u>	
<u>Mixed wastewater to treatment</u>	
Deionized water	0.004
NMP	0.009
<u>Hazardous waste</u>	
Sodium hydroxide	0.00033
Sulphuric acid	0.00022

The second manufacturing step of MWCNT NMC batteries is cathode and anode coating and drying. Data for aluminum and copper substrate were gathered from Ecoinvent 2.2. The energy use and the amount of material inputs/outputs are shown in Table 4-5.

Table 4-5 Step 2 – Materials inventory & energy use

Cathode & Anode Coating+Drying	
Total cycle time/cell	0.000004 hr
Energy	**[kWh/cell]**
Total energy /cell	0.0005 kwh
Material	**[kg/cell]**
Input	
Aluminum sheet	0.003
Copper sheet	0.005

As previously explained, the separator is a layer made of polyethylene and separates the cathode and anode. Data for the manufacture of the separator was taken from Ecoinvent 2.2 and Notter et al (Notter, Gauch et al. 2010). Step 4 is the corresponding manufacturing step which separator is used. Table 4-6 shows the energy use for manufacturing one battery cell and the amount input/output materials.

Table 4-6 Step 4– Materials inventory & energy use

Cutting	
Total cycle time/cell	0.000001 hr
Energy	**[kWh/cell]**
Total energy/cell	0.00002 kwh
Material	**[kg/cell]**
Input	
Separator	0.016
Output	
Mixed waste	
NMC	0.0002
Aluminum sheet	0.0001
Carbon black	0.0000
Graphite	0.0001
Copper sheet	0.0001
Copper sheet	0.0010

During the cell assembly, the aluminum case is used to enclose the anode, cathode, and the separator. Upstream data for the aluminum casing came from Ecoinvent 2.2. Table 4-7 shows the energy use and the amount of aluminum case used during the battery cell assembly.

Table 4-7 Step 5– Materials inventory & energy use

Electrode assembly	
Total cycle time/cell	0.0003 hr
Energy	**[kWh/cell]**
Total energy/cell	0.01 kwh
Material	**[kg/cell]**
Input	
Can / Case (aluminum)	0.004
Output	
Mixed waste	
NMC	0.0004
Total aluminum	0.0002
Total Carbon (graphite)	0.0003
Copper	0.0010
Separator	0.0002

The conductor solution between cathode and anode is called an electrolyte. The lithium-ions transfer during charging and discharging process between cathode and anode electrodes. Upstream material extraction was taken from Ecoinvent 2.2 and Notter et al (Notter, Gauch et al. 2010). The amount of electrolyte in the portable computer battery cell is shown in Table 4-8.

Table 4-8 Step 6– Materials inventory & energy use

Wetting or Filling	
Total cycle time/cell	0.0001 hr
Energy	**[kWh/cell]**
Total energy/cell	0.002 kwh
Material	**[kg/cell]**
Input	
Electrolyte	0.041

After the forming step (step 8), the battery cells and the battery management system are put in a battery pack which is called final assembly. LCI of input materials used during final assembly step, were gathered throw Ecoinvent 2.2 database. Table 4-9 shows the energy use for assembling of a MWCNT NMC cell and the amount input/output materials.

Table 4-9 Step 9– Materials inventory & energy use

Final Assembly	
Total cycle time/cell	0.017 hr
Energy	**[kWh/battery]**
Total energy/cell	0.25 kwh
Material	**[kg/battery]**
Input	
Aluminum /per module	0.021
Aluminum /per battery	0.105
Steel	0.052
Copper wiring	0.004
Aluminum	0.05
Printed circuit board	0.0001
Output	
Mixed wastewater to treatment	
Cathode input waste calculation	0.001
Anode input waste calculation	0.001
Separator	0.002
Electrolyte	0.004
Total aluminum for battery case (step 9)	0.003
Total copper per battery case (step 9)	0.0001
Total steel per battery case (step 9)	0.001

In summary, the LCI data for the manufacturing steps of the CNT NMC batteries targeted for portable computers has been effectively organized in a parametric, process-based manner. The battery contains of 6 cells. Results from the LCI indicate that energy use is extremely high in MWCNT NMC batteries manufacturing (661kWh/battery) due to the forming and testing manufacturing steps (step 8). As described in Chapter 2.1.4, the cycle time for the forming and testing step has the longest duration at between 24 to 72 hours. During the forming process, battery cells are charged and discharged repeatedly to get the desired cycle life. The resulting inventory for energy and all input and output materials to produce 1,000,000 MWCNT NMC batteries is summarized in Table 4-10.

Table 4-10 Energy and input /output materials for manufacturing computer batteries- battery includes 6 cells and total weight of 0.41kg

ENERGY	**kWh/battery**
	661 kwh
INPUT	**kg/battery**
Bases:	
Cathode active material (NMC)	0.014
Anode active material (graphite)	0.011
Carbon black	0.002
NMP	0.009
PVDF	0.001
Metals:	
Aluminum sheet	0.17
Copper sheet	0.009
Can / Case	0.015
Steel	0.052
Electrolyte	0.041
Separator	0.016
Solvents:	
Deionized water	0.004
Sodium hydroxide	0.0003
Sulphuric acid	0.0002
MWCNT	0.001
OUTPUT	**kg/battery**
Hazardous waste	0.00055
Mixed waste	0.013
Waste water treatment	0.008

Next, LCIA results of MWCNT NMC battery manufacturing are discussed. Because the major input resource in MWCNT NMC battery manufacturing is energy, the environmental impact assessment of MWCNT NMC batteries manufacturing are investigated by considering different forms of energy e.g., US grid, renewable, and the various combination of both renewable and non-renewable energy during the manufacturing.

4.4. MWCNT NMC Batteries Life Cycle Impact Assessment Results

The results in this section reflect the environmental impact of manufacture MWCNT NMC batteries for portable computers. The life cycle inventory developed in section 4.3 is used as input into SimaPro™ to perform the environmental impact assessment of the batteries. All the input materials were found in the Ecoinvent™ , while MWCNT LCI data set was built and added to the existing database (de las Casas and Li 2012, Vinayan, Nagar et al. 2012, Amarakoon 2013, Shah, Ates et al. 2014). The result of this work was developed by employing TRACI 2 impact assessment method. The input assumptions were used to run SimaPro™ for the manufacturing phase of MWCNT NMC batteries life cycle including:

- Material input — Polyvinyl fluoride has been used instead of PVDF
- Material input — Cobalt has been added as an extra element to the analysis based on a mass based assumption.
- Material input — Sodium hydroxide and hydrogen chloride were used at 50% concentration

- Electricity input —Electricity, medium voltage, at grid/US
- Hazardous waste input —disposal, hazardous waste, 25% water, to hazardous waste incineration
- Mixed wastewater input —Treatment, sewage, to wastewater treatment, class 3, where a class 3 capacity denotes a medium size municipal wastewater treatment plant
- Electricity input — Solar power has been introduced only during forming process due to high impact of electricity consumed during that step.

As discussed in section 4.3.3, energy usage during manufacture of MWCNT NMC batteries is high mostly due to extensive use of electricity. Thus, to fabricate CNT-enhanced lithium-ion batteries, different scenarios are developed by considering various types of energy e.g., US grid and mix of renewable and non-renewable energy. The four different scenarios are investigated in this study include:

- Basic scenario – 100% US grid
- Scenario 2 – using the mix of renewable and US grid (15% solar energy)
- Scenario 3 – using the mix of renewable and US grid (30% solar energy)
- Scenario 4 – using renewable energy only (100% solar energy)

4.4.1. Cumulative Energy Demand

The Cumulative Energy Demand (CED) refers to the total amount of energy used during a product life cycle including production, use, and the disposal phase (Notter, Gauch et al. 2010). In this study, the total quantity of energy during the manufacturing phase of MWCNT NMC batteries is investigated for the high EHS scenario.

Characterization results of the cumulative energy demand of MWCNT NMC battery fabrication using high EHS safety alternative with the basic energy scenario are shown in Figure 4-6. This graph illustrates the renewable and non-renewable types of energy with greatest contributions to each manufacturing process step. The contributions from each manufacturing step are sequentially ordered from the bottom of each energy type (renewable or non-renewable) to the top. The results show that the forming and testing manufacturing process step is the greatest energy-consuming step among battery fabrication steps, which holds with or without CNTs.

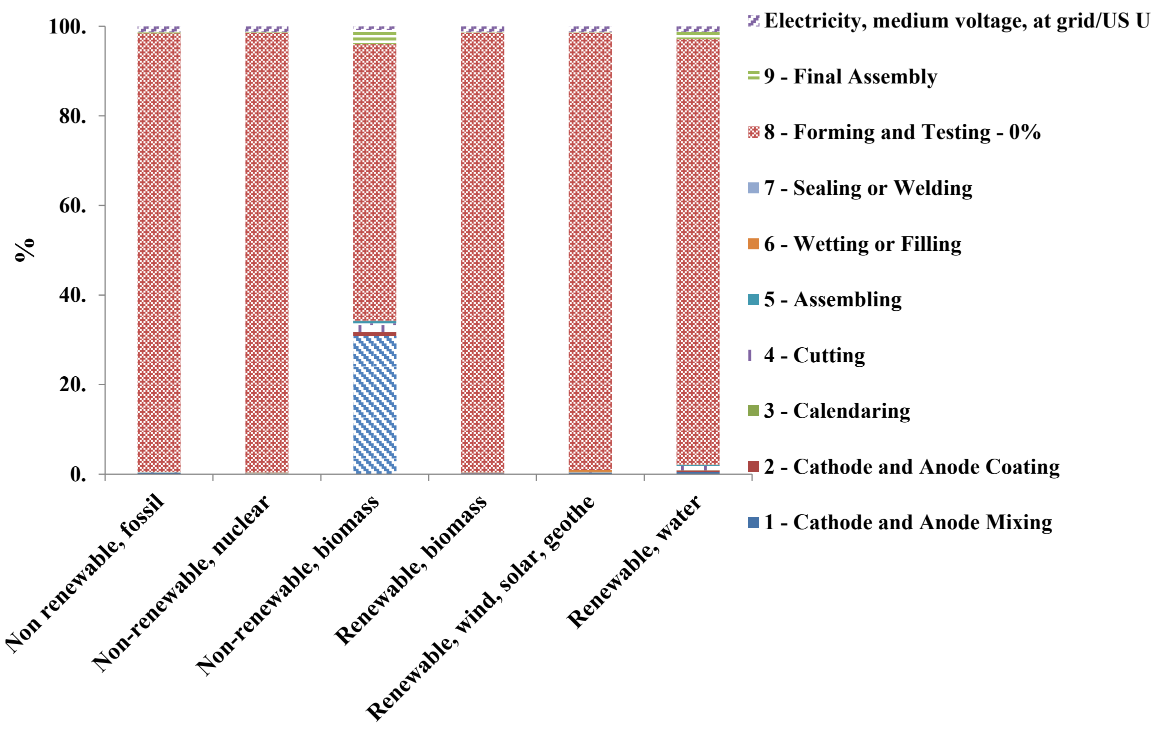


Figure 4-6 Analyzing 1 p 'Laptop MWNT Battery; Method: Cumulative Energy Demand V1.08 / Cumulative energy demand / Characterization

Figure 4-7 shows the weighting of CED of MWCNT NMC battery manufacturing. Again the results indicate that the main energy consumption during manufacture is dominated by the forming and testing step, which is mainly accomplished using fossil fuel (non-renewable energy) sources.

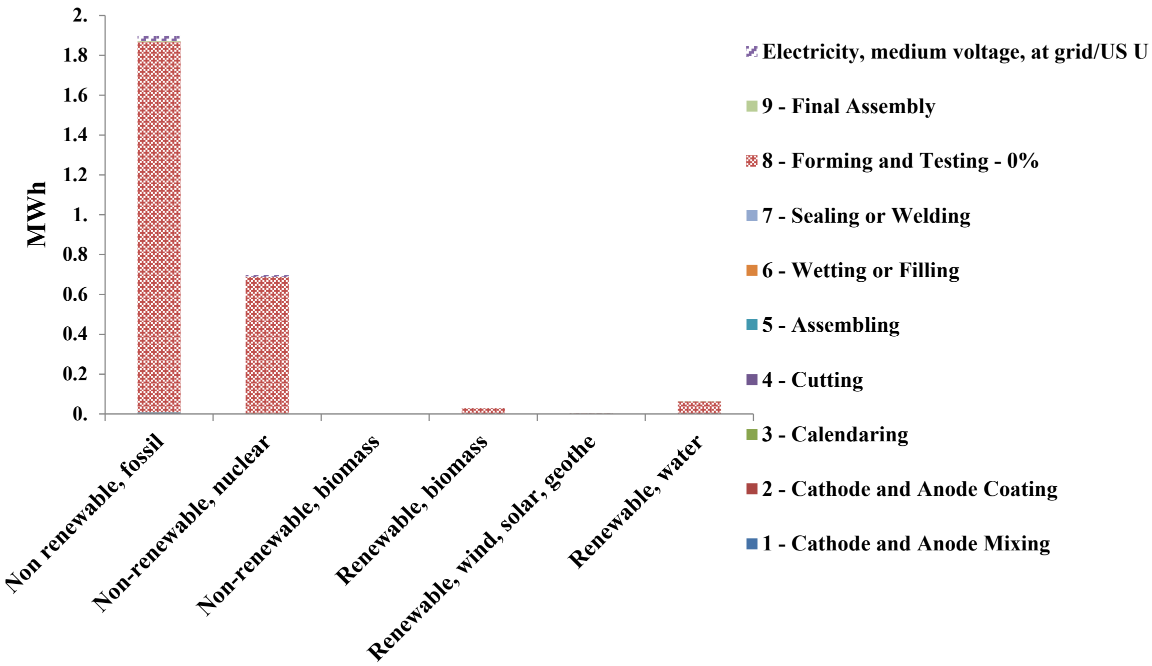


Figure 4-7 Analyzing 1 p 'Laptop MWNT Battery'; Method: Cumulative Energy Demand V1.08 / Cumulative energy demand / Weighting

Figure 4-8 compares the total CEDs for conventional NMC batteries and MWCNT NMC batteries. As explained in section 4.3.3, the CNTs employed make up 0.93% of the battery's weight. The single score total CED indicates a slightly different of energy consumption between two cases due to energy use required for MWCNT fabrication. As mentioned, the greatest amount of energy use occurs during forming and testing with energy as fossil fuels. The energy consumption difference of using fossil fuels during manufacturing of MWCNT NMC batteries is higher by 0.0257 MWh compared with conventional NMC batteries.

As explained, the total annual production of MWCNT NMC battery for computers is assumed to be 1,000,000 in 2018 (Espinoza, Erbis et al. 2014). Therefore, the difference of fossil fuel consumption energy during manufacturing of batteries with and without CNTs would be 25,700 MWh annually.

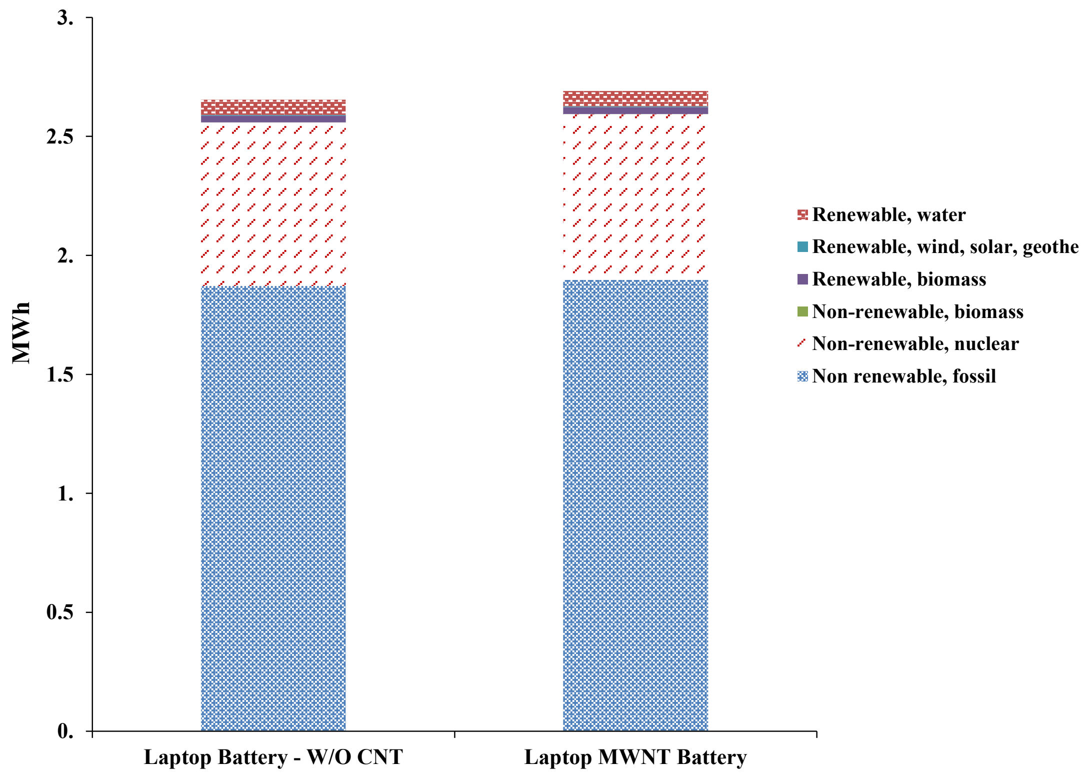


Figure 4-8 Comparing 1 p 'Laptop Battery - W/O CNT' with 1 p 'Laptop MWNT Battery'; Method: Cumulative Energy Demand V1.08 / Cumulative energy demand / Single score

4.5. TRACI Results

The complete list of impact categories examined in this study is described earlier in section 4.3. First, each impact category is discussed in detail then LCIA results of each battery manufacturing process step toward each environmental impact category are shown. The impacts by component are presented on a functional unit basis (per kg). The comparison is between conventional NMC batteries and MWCNT NMC batteries.

4.5.1. Global Warming Impacts

Having carbon dioxide (CO_2) and other greenhouse gases in the atmosphere may affect the climate change and increase the earth temperatures. The potential heat relative to CO_2 that is contributed to the atmosphere by different chemicals is called global warming potential (GWP) and is measured by the mass of a global warming gas released to air, adjusted by a GWP equivalency factor (Amarakoon 2013), with units of CO_2 equivalents. Table 4-11 presents the GWP by battery fabrication step during the production and manufacturing phases of MWCNT NMC batteries and conventional NMC batteries. GWP of electricity use considering high and low EHS scenarios during manufacture of MWCNT NMC batteries and conventional NMC batteries are listed. The results indicate forming and testing step has the greatest contribution toward GWP.

Table 4-11 Global Warming Potential by battery process break down comparing two batteries

Process steps	MWCNT NMC batteries (kg CO_2 eq)	NMC batteries (kg CO_2 eq)
1-Cathode and Anode Mixing	1.0541	0.9697
2-Cathode and Anode Coating	0.3118	0.3117
3-Calendaring	0.0004	0.0004
4-Cutting	0.8026	0.8026
5-Assembling	0.2468	0.2468
6-Wetting or Filling	0.3626	0.3626
7-Sealing or Welding	0.0361	0.0361
8-Forming and Testing	569.4003	569.4003
9-Final Assembly	1.5154	1.5154
Total	**573.729**	**573.648**
Electricity, medium voltage, at grid/US U	7.6911	2.3071

4.5.2. Acidification Potential

The increased acidity of soil and water is caused by air acidification. To determine the potential acidification impacts from inorganic air emissions across the manufacture of MWCNT NMC batteries, the potential acidification for manufacturing processes are compared for MWCNT NMC and conventional NMC battery manufacturing. The acidification impact units are hydrogen ion-molar equivalents produced per kilogram of emission (H+ moles eq) (Amarakoon 2013). Table 4-12 presents the potential acidification by battery fabrication steps during production and manufacturing phases of

MWCNT NMC batteries and conventional NMC batteries. The potential acidification of electricity use considering high and low EHS scenarios during manufacturing of MWCNT NMC and conventional NMC batteries are also shown. The results show the acidification impact is dominated by forming and testing process step due to high energy consumption.

Table 4-12 Acidification potential by battery process break down comparing two batteries

Process steps	MWCNT NMC batteries (H+ moles eq)	NMC batteries (H+ moles eq)
1-Cathode and Anode Mixing	0.3328	0.3069
2-Cathode and Anode Coating	0.7859	0.7859
3-Calendaring	0.0001	0.0001
4-Cutting	0.1909	0.1909
5-Assembling	0.0641	0.0641
6-Wetting or Filling	0.0902	0.0902
7-Sealing or Welding	0.0128	0.0128
8-Forming and Testing	201.736	201.736
9-Final Assembly	0.4776	0.4776
Total	**203.691**	**203.669**
Electricity, medium voltage, at grid/US U	2.725	0.817

4.5.3. Eutrophication Potential

The potential impact of regional water quality from chemicals and emissions e.g., nitrogen and phosphorus called eutrophication. The units of the weighting values in this impact category are nitrogen equivalents per kilogram of emission (kg N eq) (Amarakoon

2013). Table 4-13 compares eutrophication for MWCNT NMC batteries and traditional NMC batteries. The eutrophication comparison of their corresponding EHS scenarios and electricity use (high and low) is also shown. The results indicate forming and testing step has the greatest contribution toward eutrophication.

Table 4-13 Eutrophication potential by battery process break down comparing two batteries

Process steps	MWCNT NMC batteries (kg N eq)	NMC batteries (kg N eq)
1-Cathode and Anode Mixing	0.0055	0.0047
2-Cathode and Anode Coating	0.0394	0.0394
3-Calendaring	1.42E-06	1.42E-06
4-Cutting	0.0029	0.0029
5-Assembling	0.0009	0.0009
6-Wetting or Filling	0.0027	0.0027
7-Sealing or Welding	0.0001	0.0001
8-Forming and Testing	2.1892	2.1892
9-Final Assembly	0.01099	0.01099
Total	**2.252**	**2.251**
Electricity, medium voltage, at grid/US U	0.0296	0.0089

4.5.4. Ozone Depletion

The harmful radiation from the sun is filtered out by the ozone layer. Therefore, it is critical to prevent releasing chemicals, and emissions that may result in destroying the ozone stratospheric layer. Impact scores are based on the identity and amount of ozone-depleting chemicals (ODC) released to air per functional unit (kg CFC-11 eq)

(Amarakoon 2013). Table 4-14 lists the ODC by battery fabrication steps during production and manufacturing phases of MWCNT NMC batteries and the electricity use including the high EHS scenario for MWNCT NMC batteries versus low EHS scenario for conventional NMC batteries. The results indicate the forming and testing step has the greatest contribution toward ODC.

Table 4-14 Ozone depletion potential by battery process break down comparing two batteries

Process steps	MWCNT NMC batteries (kg CFC-11 eq)	NMC batteries (kg CFC-11 eq)
1-Cathode and Anode Mixing	8.38E-08	8.12E-08
2-Cathode and Anode Coating	2.085E-08	2.08E-08
3-Calendaring	9.771E-12	9.77E-12
4-Cutting	5.090E-08	5.09E-08
5-Assembling	1.391E-08	1.39E-08
6-Wetting or Filling	2.523E-08	2.5E-08
7-Sealing or Welding	9.591E-10	9.59E-10
8-Forming and Testing	1.513E-05	1.51E-05
9-Final Assembly	8.981E-08	8.98E-08
Total	**1.535E-05**	**1.535E-05**
Electricity, medium voltage, at grid/US U	2.03E-07	6.1E-08

4.5.5. Ecological Toxicity Potential

Ecological toxic potential equals the ecological toxicity potential (ETP) by the amount of the ecologically toxic chemical (ETC) released to the air, soil, or water (kg) per functional unit and is shown by (kg 2,4-D eq) (Rosenbaum, Bachmann et al. 2008). The ecological potential is estimated based on the following formula:

$$IS_{ETP} = CF_{ETP} + CF_{ETC} \tag{1}$$

where IS_{ETP} equals the impact score for ecological toxicity of the chemical, CF_{ETP} equals the ecological toxicity potential, and CF_{ETC} equals the amount of the ecologically toxic chemical (ETC) released to the air, soil, or water (Rosenbaum, Bachmann et al. 2008) of electricity use considering high and low EHS scenarios during manufacture of MWCNT NMC and conventional NMC batteries are also shown.

Table 4-15 presents the ecological toxicity potential impact scores by battery manufacturing process. The ecological toxic potential of electricity use considering high and low EHS scenarios during manufacture of MWCNT NMC and conventional NMC batteries are also shown. The results indicate that the forming and testing step has the greatest contribution toward ecological toxicity potential.

Table 4-15 Ecological toxicity potential by battery process break down comparing two batteries

Process steps	MWCNT NMC batteries (kg 2,4-D eq)	NMC batteries (kg 2,4-D eq)
1-Cathode and Anode Mixing	13.919	13.314
2-Cathode and Anode Coating	41.5301	41.5301
3-Calendaring	0.0011	0.0011
4-Cutting	6.0588	6.0588
5-Assembling	1.6496	1.6496
6-Wetting or Filling	1.56413	1.56413
7-Sealing or Welding	0.10469	0.10469
8-Forming and Testing	1665.591	1665.591
9-Final Assembly	16.5482	16.5482
Total	**1746.966**	**1746.364**
Electricity, medium voltage, at grid/US U	22.496	6.749

Characterization results of the overall environmental impacts of MWCNT NMC batteries and conventional NMC batteries are shown in Figure 4-9. The impacts from each battery (with /without MWCNTs) are represented for every impact category. As shown in Figure 4-9, the environmental impacts of MWCNT NMC battery manufacturing are more than 1% higher for all impact categories. It is expected the environmental impact differences during batteries (with CNTs / without CNTs) manufacturing processes results due to existence of CNTs in the process.

To explore this more closely, an environmental impact analysis for the cathodes with MWCNTs and the cathodes without MWCNTs in batteries are conducted. All of the input materials and resources during cathode manufacturing process in both cases are considered to be equal, except for the addition of MWCNTs and the associated energy consumption for the high EHS scenario during the manufacturing process. The results are shown in Figure 4-10.

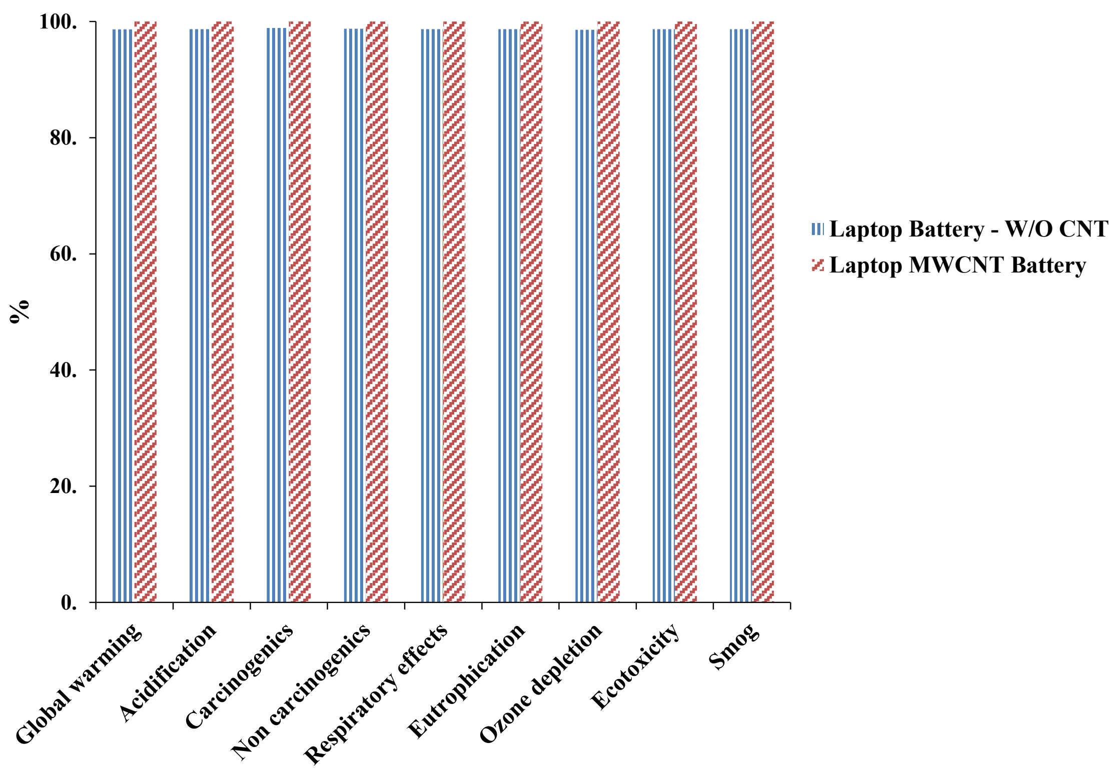


Figure 4-9 Comparing 1 p 'Laptop Battery - W/O CNT' with 1 p 'Laptop MWNT Battery'; Method: TRACI 2 V3.03 / Characterization

As expected, all the environmental impacts in different impact categories in MWCNT NMC cathodes are higher than environmental impacts of traditional cathodes manufacturing during mixing process and caused by MWCNTs. The comparison results in Figure 4-10 indicates ozone depletion is the most affected environmental impact category among the other impact categories and is almost higher by 20% in MWCNT NMC batteries manufacturing mixing step. This happens because of the need for different materials and different amount of energy during manufacturing of MWCNTs comparing with manufacturing of carbon black.

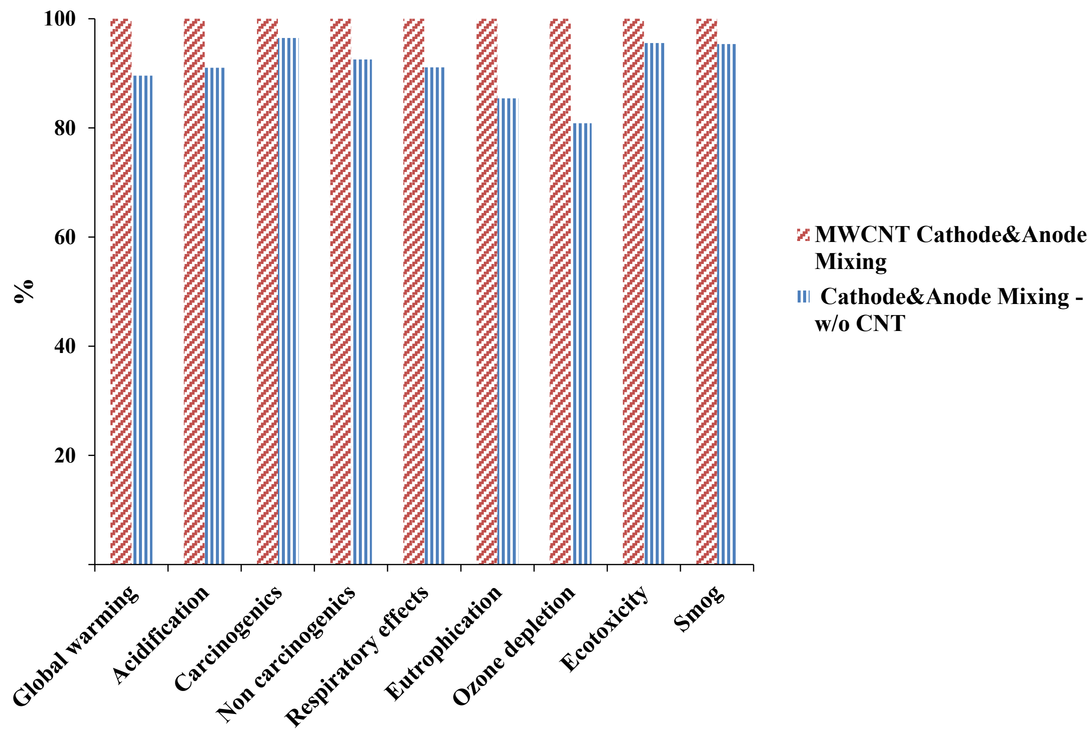


Figure 4-10 Comparing 1 p '1 - Cathode and Anode Mixing' with 1 p '1 - Cathode and Anode Mixing - w/o CNT';Method: TRACI 2 V3.03 / Characterization

4.6. Sustainable Nano-Manufacturing

The amount of energy usage during manufacture of MWCNT NMC batteries is high mostly due to extensive electricity use during forming and testing manufacturing step. Thus, to make CNT-enhanced lithium-ion battery manufacturing process more sustainable, different battery manufacturing scenarios are developed by considering using different combination of US grid and renewable energy during MWCNT NMC battery manufacturing including:

- Basic scenario – 100% US grid
- Scenario 2 – using the mix of renewable and US grid (15% solar energy)
- Scenario 3 – using the mix of renewable and US grid (30% solar energy)
- Scenario 4 – using renewable energy only (100% solar energy)

Figure 4-11 illustrates the comparison of CED results for manufacture of the MWCNT NMC battery for US grid and different mixtures of US grid and renewable energy (solar energy) during battery manufacturing. This graph indicates, although the amount of energy use during battery manufacture remains the same, the total embodied energy of the battery decreases considerably. For instance, replacing energy from the US grid with renewable energy (solar energy) reduces total energy use by 280 KWh and 450 KWh per battery for having 15% and 30% solar energy in the system. Scenario 4 is discussed separately.

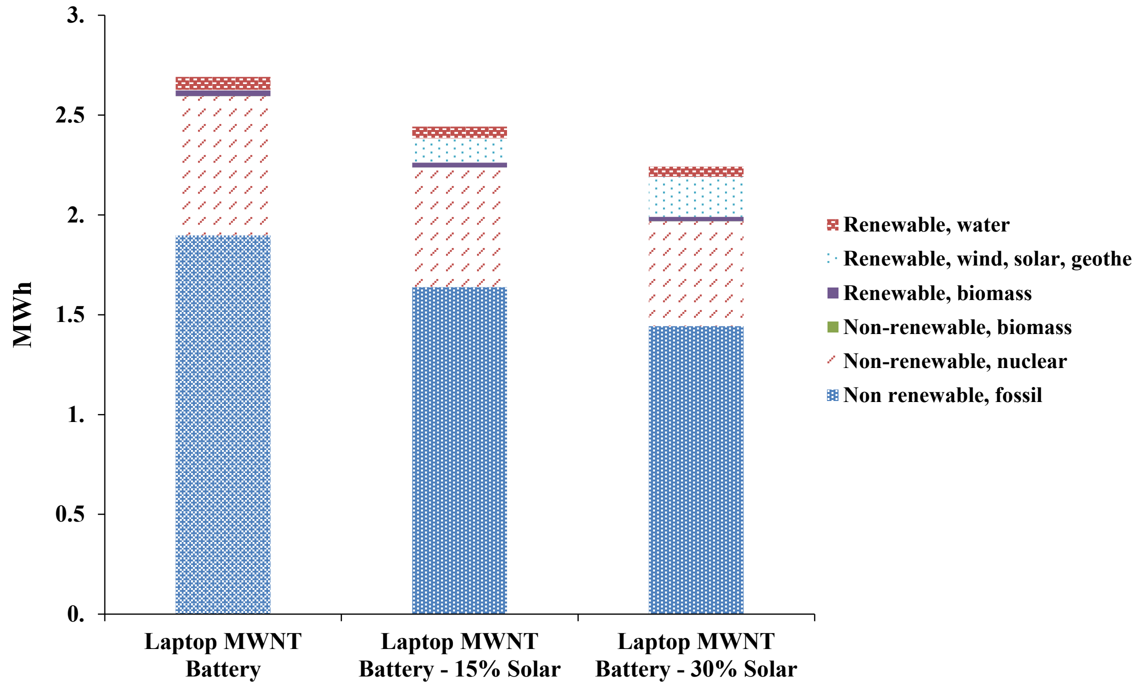


Figure 4-11 Comparing 1 p 'Laptop MWNT Battery', 1 p 'Laptop MWNT Battery - 15% Solar' and 1 p 'Laptop MWNT Battery - 30% Solar'; Method: Cumulative Energy Demand V1.08 / Cumulative energy demand / Single score

The characterization results of MWCNT NMC battery manufacture that compares different forms of energy during forming and testing is shown in Figure 4-12. The results indicate that replacing US grid by renewable energy reduces environmental burdens in all categories. For instance, using the mix of US grid and 30% solar energy decreases the global warming, ecotoxicity, and ozone depletion by 25%, 22%, and 15%, respectively during manufacturing of one MWCNT NMC battery.

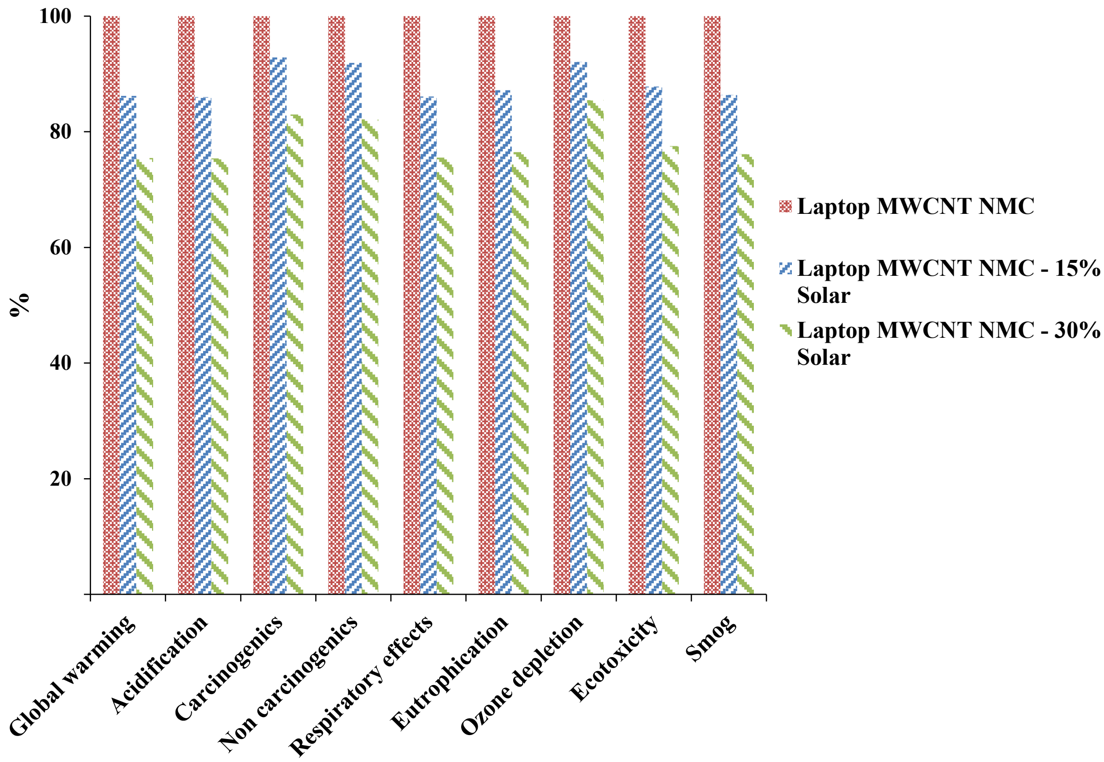


Figure 4-12 Comparing 1 p 'Laptop MWCNT NMC Battery', 1 p 'Laptop MWCNT NMC Battery - 15% Solar' and 1 p 'Laptop MWCNT NMC Battery - 30% Solar'; Method: TRACI 2 V3.03 / Characterization

Figure 4-13 shows the environmental burden comparisons of MWCNT NMC battery manufacturing using US grid and 100% renewable energy (solar energy). As experts say, 100% solar energy during manufacturing process is so optimistic and is not likely to happen any time soon. However, if 100% renewable solar energy were possible for manufacture of MWCNT NMC batteries, then the environmental impacts decrease dramatically compared with the base case scenario (100% US grid). Global warming, acidification, and respiratory effects are the environmental impact categories that show greatest decreases.

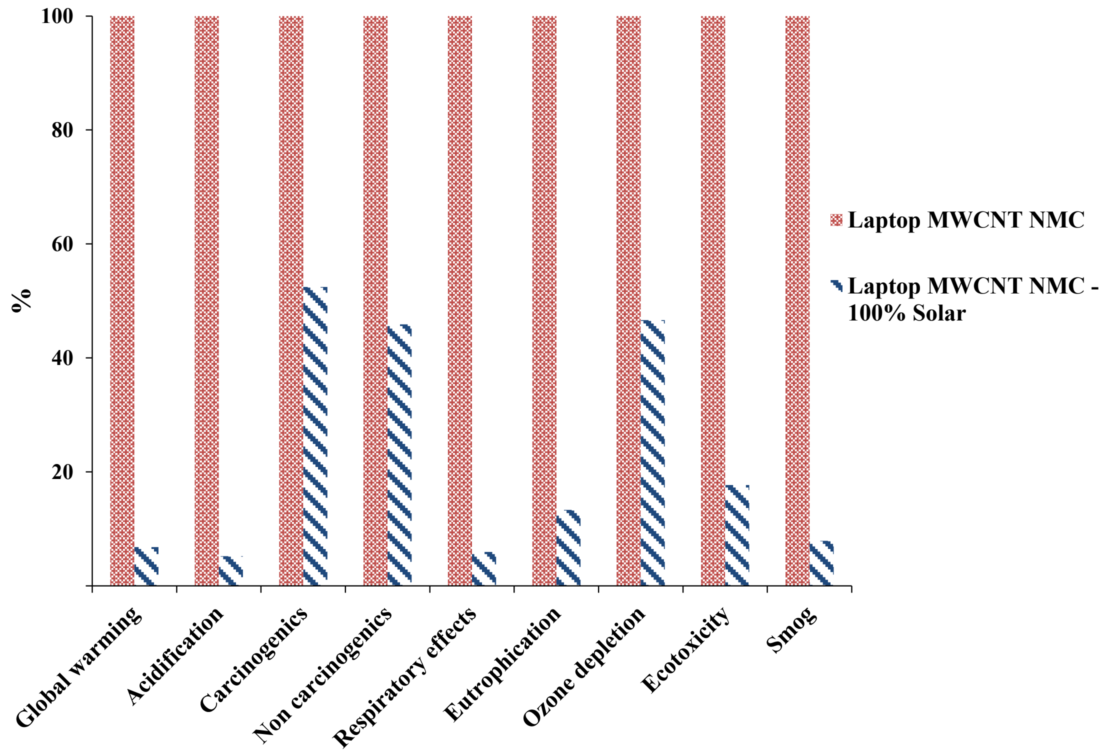


Figure 4-13 Comparing 1 p 'Laptop MWCNT NMC Battery' with 1 p 'Laptop MWCNT NMC Battery - 100% Solar'; Method: TRACI 2 V3.03 / Characterization

Using renewable energy (solar energy) during the manufacture process of MWCNT NMC batteries not only decreases the environmental burdens (Figure 4-12), but also it significantly decreases the total embodied energy of the battery (Figure 4-11). However, use of renewable energy could be costly with increases to the total manufacturing unit cost. Table 4-16 shows the total unit cost (total cost of a computer battery) for various EHS scenarios by consideration of different combinations of US grid and renewable energy. The results indicated the total manufacturing unit cost increased by approximately $20 for different EHS scenarios if using 100% solar renewable energy during battery manufacturing.

T**able 4-16** Total computer battery unit cost by different energy combination

	Total unit cost per – Computer battery		
Energy mix	**LOW EHS**	**Medium EHS**	**High EHS**
100% US grid	$152	$155	$161
US grid and 15% solar energy	$155	$158	$164
US grid and 30% solar energy	$159	$161	$168
100 % solar energy	$171	$174	$180

CHAPTER 5 MULTI-CRITERIA DECISION ANALYSIS

To determine and select the best choice (from decision makers' perspectives) among different alternatives (various types of produced batteries), Analytical Hierarchy Process (AHP) technique is used (Beccali, Cellura et al. 2003, Tudela, Akiki et al. 2006, Wang, Jing et al. 2009, Zopounidis and Pardalos 2010, Zopounidis and Doumpos 2013). AHP approach comprises 3 different components: overall objective goal, decision makers' preferred criteria and sub-criteria, and decision alternatives (Kablan 2004, Saaty 2008, Sipahi and Timor 2010). AHP uses the judgment of stakeholders to form and prioritize the multiple criteria to resolve and select the best solution. Once the decision makers' interests are identified, they are rated according to each stakeholder preferences by conducting paired-wise comparisons.

In this study, 4 different stakeholders are considered: manufactures, consumers, regulators, and the environmental analysts while various criteria are categorized into production cost, power density of the product, occupational exposure during manufacture, product life, and disposal of Personal Protective Equipment (PPE) hazardous waste during manufacturing. Decision alternatives include conventional NMC batteries (no CNTs) versus MWCNT NMC batteries with different safety standards (low, medium, and high safety standards). Figure 5-1 illustrates APH methodology in details.

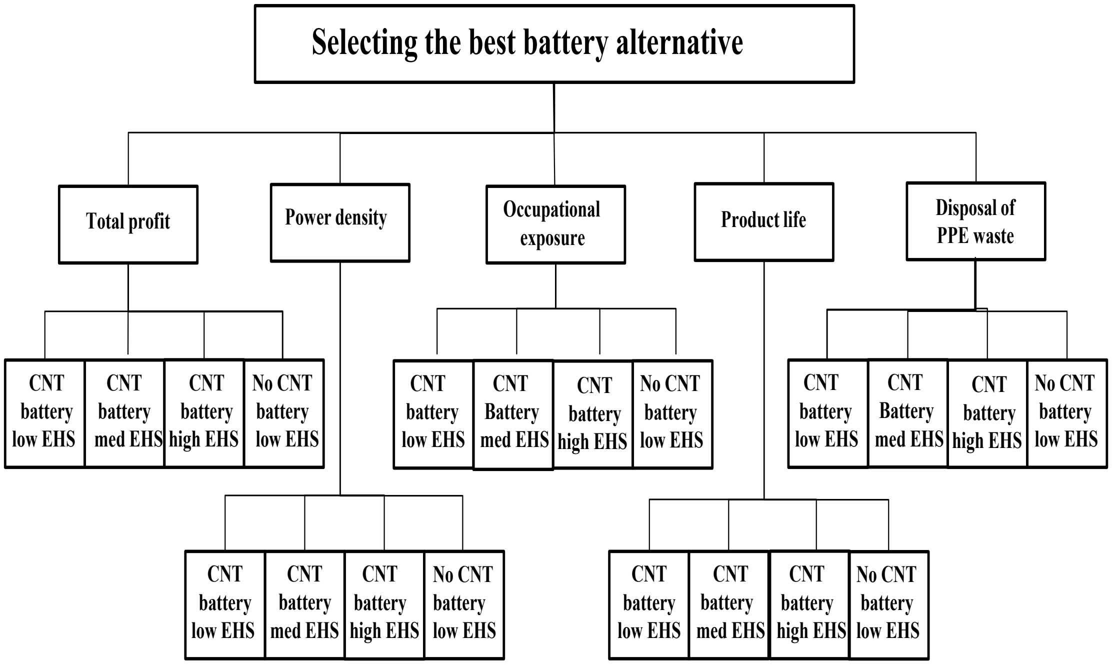


Figure 5-1 Hierarchy of attributes and decision alternatives

To develop the comparison matrices with calculated weights by using the AHP preference scale, the numerical rating concept is used to compare the factors or criteria. The numerical rating table is shown below (Table 5-1).

Table 5-1 Numerical rating preferences

Intensity of importance	Numerical rating
Extremely more important	9
Very strongly more important	7
Strongly more important	5
Moderately more important	3
Equally more important	1

Relative to other alternatives, each criterion is rated based on the experts' opinion obtained through surveys to fulfill the stakeholders' preferences. For each decision maker, the comparison matrix is formed separately.

Table 5-2, Table 5-3, Table 5-4, and Table 5-5 illustrate the comparison matrix for the assumed stakeholders: manufactures, consumers, regulators, and the environmental analyst group for both satellites and computers.

Table 5-2 Manufacturers' comparison matrix for satellites & computers

	Production cost	Power density	Occupational exposure	Product life	Disposal of PPE waste
Production cost	1	3	7	5	9
Power density	0.33	1	7	3	9
Occupational exposure	0.14	0.14	1	0.20	7
Product life	0.20	0.33	5	1	9
Disposal of PPE waste	0.11	0.11	0.14	0.11	1

Table 5-3 Consumers' comparison matrix for satellites & computers

	Production cost	Power density	Occupational exposure	Product life	Disposal of PPE waste
Production cost	1	0.33	9	7	0.33
Power density	3	1	9	3	3
Occupational exposure	0.11	0.11	1	0.11	0.14
Product life	0.14	0.33	9	1	5
Disposal of PPE waste	3	0.33	7	0.20	1

Table 5-4 Regulators' comparison matrix for satellites & computers

	Production cost	Power density	Occupational exposure	Product life	Disposal of PPE waste
Production cost	1	1	0.11	0.33	0.14
Power density	1	1	0.11	0.33	0.14
Occupational exposure	9	9	1	7	5
Product life	3	3	0.14	1	0.33
Disposal of PPE waste	7	7	0.20	3	1

Table 5-5 Environmental analysts' comparison matrix for satellites & computers

	Production cost	Power density	Occupational exposure	Product life	Disposal of PPE waste
Production cost	1	1	0.20	0.33	0.11
Power density	1	1	0.20	0.33	0.11
Occupational exposure	5	5	1	0.20	0.14
Product life	3	3	0.20	1	0.11
Disposal of PPE waste	9	9	7	9	1

The comparison matrices are then normalized and averaged. By weighting out the results, the criteria priority ranking matrices (preference matrices) for each decision maker are formed and used to calculate the stakeholders' benefit. Table 5-6 shows the decision makers' preference matrices. The criteria preferences are ordered from high priority to low in the Tables below.

Table 5-6 Stakeholders' criteria priority ranking matrices in satellites & computers

(a) Manufacturers

1- Production cost	0.47
2- Power density	0.27
3- Product life	0.16
4- Occupational exposure	0.08
5- Disposal of PPE hazardous waste	0.03

(b) Consumers

1- Power density	0.35
2- Production cost	0.24
3- Product life	0.21
4- Disposal of PPE hazardous waste	0.18
5- Occupational exposure	0.02

(c) Regulators

1- Occupational exposure	0.57
2- Disposal of PPE hazardous waste	0.24
3- Product life	0.10
4- Power density	0.04
4- Production cost	0.04

(d) Environmental analyst group

1-Disposal of PPE hazardous waste	0.65
2- Occupational exposure	0.15
3- Product life	0.10
4- Power density	0.05
4- Production cost	0.05

After developing the preference matrices, the decision matrix for different alternatives is constructed by running the model for different safety standard scenarios with and without CNTs. Table 5-7 and Table 5-8 show the decision matrices for the satellites and the computers, respectively. Having CNTs in the manufacturing area with low EHS safety standards causes higher rate of occupational exposure. In the manufacturing environment with high EHS safety standards, the chance of exposure to CNTs is low due to highly protected environment. The rate of disposal of PPE hazardous waste in medium safety standard area is considered higher than that in low EHS safety standards because of the higher mass of PPEs used in the medium safety standard area. However, the rate of disposal of PPE hazardous waste in the high safety standard manufacturing environment is considered to be low because PPE hazardous waste are assumed to be disposed. Product life assumes higher in the NMC batteries with CNTs due to positive impacts of CNTs in emerging products. Tables below show the decision matrices for both satellites and computers for NMC batteries with / without MWCNTs.

Table 5-7 Satellites criteria/decision matrix

	With CNT			**Without CNT**
	Low EHS	**Medium EHS**	**High EHS**	**Low EHS**
Production cost	\$12,662	\$12,916	\$13,488	\$11,478
Power density	1800 W/kg	1800 W/kg	1800 W/kg	200 W/kg
Occupational exposure (scale)	8 out of 10	4 out of 10	1 out of 10	0 out of 10
Product life	4 yrs	4 yrs	4 yrs	1 yr
Disposal of PPE waste (scale)	5 out of 10	9 out of 10	2 out of 10	0 of 10

Table 5-8 Computers criteria/decision matrix

	With CNT			Without CNT
	Low EHS	Medium EHS	High EHS	Low EHS
Production cost	\$152	\$155	\$162	\$146
Power density	200 W/kg	200 W/kg	200 W/kg	160 W/kg
Occupational exposure (scale)	8 out of 10	4 out of 10	1 out of 10	0 out of 10
Product life	6 yrs	6 yrs	6 yrs	3 yr
Disposal of PPE waste (scale)	5 out of 10	9 out of 10	2 out of 10	0 of 10

To determine the benefit matrix (overall goal) for each decision maker for satellites and computers, the relative preference matrix of each stakeholder (Table 5-6) must be multiplied by the normalized decision value matrices (Table 5-9 and Table 5-10).

Table 5-9 Satellites criteria/decision normalized value matrix

	With CNT			Without CNT
	Low EHS	Medium EHS	High EHS	Low EHS
Production cost	0.251	0.256	0.267	0.227
Power density	0.321	0.321	0.321	0.036
Occupational exposure (scale)	0.615	0.308	0.077	0
Product life	0.308	0.308	0.308	0.077
Disposal of PPE waste (scale)	0.313	0.563	0.125	0

Table 5-10 Computers criteria/decision normalized value matrix

	With CNT			Without CNT
	Low EHS	**Medium EHS**	**High EHS**	**Low EHS**
Production cost	0.247	0.252	0.263	0.239
Power density	0.263	0.263	0.263	0.211
Occupational exposure (scale)	0.615	0.308	0.077	0
Product life	0.286	0.286	0.286	0.143
Disposal of PPE waste (scale)	0.313	0.563	0.125	0

The profile benefit matrices (Tables 19&20) are developed based on the following formula (equation 7).

$$Benefit\ Matrix = \frac{\sum_i (W_j^+ * X_{ij}^+)}{\sum_i (W_j^- * X_{ij}^-)} \tag{7}$$

where X_{ij} is an element in criteria decision matrices (Table 5-9 and Table 5-10) and W_j is an element in Stakeholders' criteria priority ranking matrices (Table 5-6). The positive parameters are the desirable criteria while the negative parameters are the non-desirable criteria according to stakeholders' perspectives.

Final results (Table 5-11and Table 5-12) determine the most beneficial type of satellite and computer battery for each stakeholder. The largest value in terms of priority weight is the most desirable choice for the relative decision maker.

Table 5-11 Decision makers' benefit matrices for satellites

NMC batteries		Manufacturers	Consumers	Regulators	Environmental analysts
With CNT	Low EHS	0.35	0.60	0.09	0.12
	Medium EHS	0.38	0.49	0.11	0.09
	High EHS	0.43	0.84	0.38	0.31
Without CNT	Low EHS	0.12	0.31	0.80	0.73

Table 5-12 Decision makers' benefit matrices for computers

NMC batteries		Manufacturers	Consumers	Regulators	Environmental analysts
With CNT	Low EHS	0.32	0.55	0.08	0.11
	Medium EHS	0.35	0.45	0.11	0.08
	High EHS	0.47	0.78	0.36	0.29
Without CNT	Low EHS	0.20	0.59	1.43	1.30

The decision makers' benefit matrices indicate that the best option for the manufactures (in satellites and computers) is to produce MWCNT NMC batteries with high EHS safety standards followed by medium and low safety standard scenario. The least preferred option for the manufacturer is to focus on producing the NMC batteries with no CNTs. Similarly, identifying the most desired option for the environmental analyst group (in satellites and computers) is producing NMC batteries with no CNTs followed by CNT NMC batteries considering high, low, and medium EHS safety standards in that order.

5.1. Benefit-Cost Ratio Analysis

To develop the benefit-cost ratio analysis, the calculated benefit matrices relative to each stakeholder should be normalized and divided to the total production cost of different EHS safety standard scenarios. Table 5-13 shows the benefit-cost ratio of MWCNT NMC batteries for both satellites and computers. In order to compare the cost-benefit results of stakeholders' perspectives, different annual production volumes are considered in the analysis. For satellites, the targeted stakeholders are manufacturers while regulators are selected to analyze for the computers.

Table 5-13 Benefit-cost ratio-manufacturers for satellites/regulators for computers

Satellites / Computers				
Total production volume / yr	**Benefit-cost-ratio (With CNT-low EHS)**	**Benefit-cost-ratio (With CNT-med EHS)**	**Benefit-cost-ratio (With CNT-high EHS)**	**Benefit-cost-ratio (No CNT-low EHS)**
100 /100,000	1.22/ 0.19	1.11/ 0.24	1.13/ 0.68	0.46/ 3.06
200 /200,000	1.16/ 0.19	1.13/ 0.23	1.19/ 0.68	0.44/ 3.05
300 /500,000	1.15/ 0.18	1.13/ 0.23	1.23/ 0.68	0.41/3.05
400 /1M	1.12/ 0.17	1.14/ 0.22	1.23/ 0.69	0.43/ 3.04
500 /2M	1.12/ 0.17	1.14/ 0.21	1.23/ 0.69	0.42/ 3.04
1,000 /3M	1.13/ 0.16	1.18/ 0.21	1.29/ 0.69	0.36/ 3.03
1,500 /4M	1.10/ 0.16	1.15/ 0.21	1.26/ 0.69	0.42/ 3.03
2,000 /5M	1.09/ 0.16	1.15/ 0.21	1.26/ 0.69	0.42/ 3.03
2,500 /10M	1.09/ 0.16	1.15/ 0.21	1.26/ 0.69	0.42/ 3.03
3,000 /20M	1.07/ 0.16	1.21/ 0.21	1.24/ 0.69	0.41/ 3.03

Figure 5-2 and Figure 5-3 show benefit-cost ratio result for manufacturer in satellites and regulators in computers, respectively.

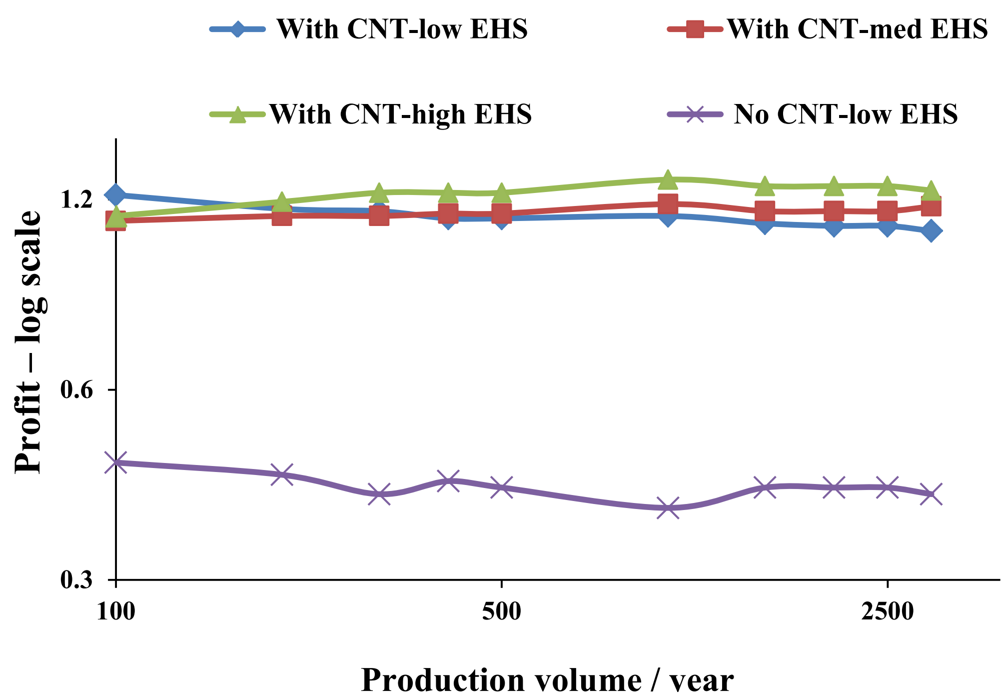


Figure 5-2 Log – log benefit-cost ratio scale for manufactures in satellites

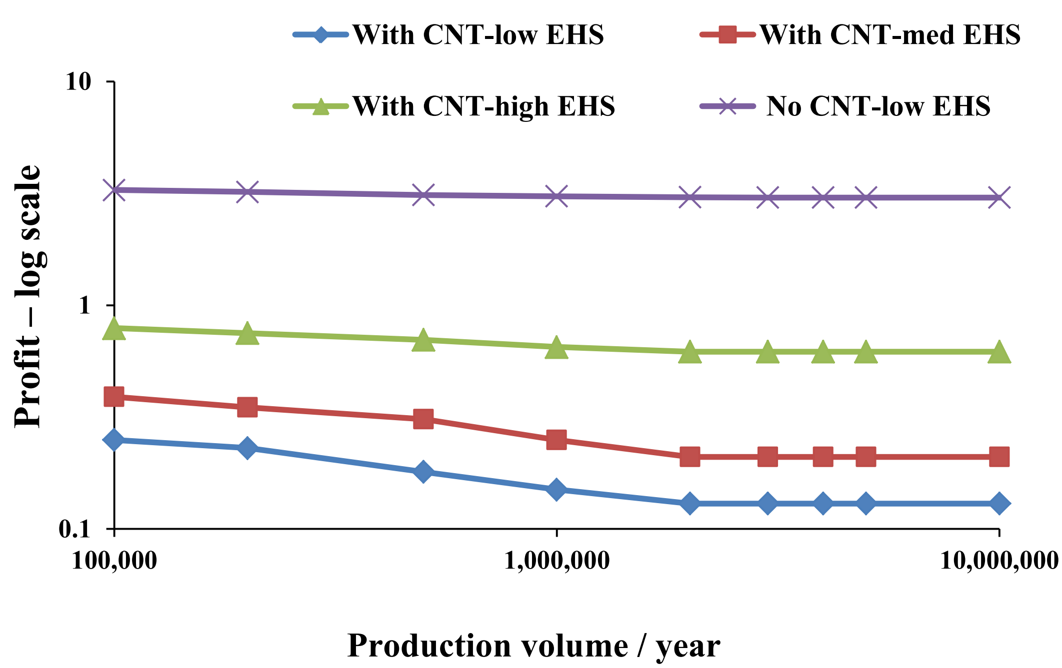


Figure 5-3 Log – log benefit-cost ratio scale for regulators in computers

As mentioned, the results identify the most desirable product for each stakeholder for different production volume. Figure 5-2 indicates producing CNT satellite batteries with high safety standards is the best option for the manufactures, followed by CNT batteries with medium and low safety standard options in long run. For regulators, the best option is to select computer batteries with no CNTs and low EHS scenario. The second best choice for the regulators is CNT batteries with high safety standard options followed by the medium and low EHS standards.

CHAPTER 6 CONCLUSIONS AND FUTURE WORK

6.1. Conclusions

The economic and the environmental health and safety tradeoffs and associated cost of exposure prevention during the mass production of carbon-nanotube-enhanced lithium-ion batteries (MWCNT NMC batteries) in satellites and computers has been explored. To conduct the analysis, a comprehensive literature review of lithium-ion batteries and CNTs properties was investigated. A particular combination of lithium-ion cell-chemistry (NMC) and carbon nanotube types (MWCNTs) was selected for the satellite and computer battery, based on developments performed by researches in the Center for High-rate Nanomanufacturing.

A process-based cost model (PBCM) was developed to estimate manufacturing scale-up of MWCNT NMC batteries, while exploring the manufacturing unit costs of alternative safety levels (low, medium, and high EHS scenarios). With the uncertainty and possible risk associated with exposure to engineered-nanoparticles, the advantage of applying PBCM lies in identification of the cost drivers for alternative processes that can result in more responsible and safer manufacturing. By combining the process-based cost model with design of experiment based analysis, the effects of process yield, cycle time, personal protective equipment (PPE) disposal costs, energy costs and MWCNT costs were explored.

Energy is shown to be a major driver of manufacturing cost, particularly for the forming and testing step. Process changes to reduce energy consumption could include recapturing the discharge energy during the forming and testing process to utilize elsewhere in the battery manufacturing facility. The use of renewable energy could also be explored to determine the effects on unit cost as well as on related environmental impacts. Inclusion of MWCNTs to fabricate nano-enabled batteries might well require higher levels of EHS safety and with respect to energy consumption throughout the process, only the higher levels of ventilation would result in any significant energy increases.

The use of MWCNT in batteries results in significant enhancements (e.g., increased specific energy by 20%, improved battery life by 100%, and longer run time by 25%), and yet the resulting cost increase for inclusion of MWCNTs appears be to relatively small for the base case of low EHS: 4% increase for computer MWCNT batteries and 7% increase for satellite MWCNT batteries compared with comparable non-MWCNT batteries. When comparing the cost differential of the high EHS manufacturing scenario batteries with non-MWCNT batteries, more significant increases result: 12% higher for computer MWCNT batteries and 16% higher for satellite MWCNT batteries, compared with non-MWCNT batteries. There are several ways to assess whether these increases are worthwhile to stakeholders. For end users or manufacturers, it is notable that when comparing the cost of a unit of energy density for batteries with and without CNTs, the cost decreases from ~$0.45 per Wh/kg (for batteries without CNTs) to $0.40 per Wh/kg for MWCNT-enhanced computer batteries. Further, as technical experimentation shows that the lifetime of MWCNT NMC computer batteries will increase by 100% compared with traditional NMC batteries, it useful to compare an annualized cost of use. Just as LED light bulbs cost more but last longer, an annualized cost for MWCNT computer batteries is spread over a 6 year lifetime as opposed 3 years period for computer batteries without MWCNTs. Considering 10% interest rate on initial investment, the annualized cost of a MWCNT computer battery is \$21 as opposed to \$34 for a computer battery without MWCNTs. Similarly considering the life of a satellite battery with MWCNT to be 4 years as opposed to 2 years for its counterpart without MWCNTs, the annualized unit cost drops from \$6,880 to \$4,213. Although the MWCNT-enabled batteries are more expensive, they are less expensive on an annualized basis, considering their value-added properties for the longer lifetime.

The costs associated for implementing higher levels of EHS protection during manufacture may also be readily accepted by manufacturers, given the cost of potential future liabilities. This study shows that the manufacturing unit cost increases by ~6% from the base case (low EHS) compared with the high EHS scenario for both computer and satellite applications. The liability costs, if MWCNT regulations were imposed or retroactive, would surely be higher than the cost of implementing more responsible industrial hygiene practices. Thus by taking preventative action to avoid the potential health and environmental consequences of MWCNT in the manufacturing area, it is highly likely to result in lower economic risk.

Life Cycle Assessment (LCA) of the traditional NMC batteries and the MWCNT NMC batteries in portable computers was performed by employing the Ecoinvent 2.2 inventory database and considering two impacts assessment methods: Cumulative Energy Demand (CED) and TRACI 2. LCA of manufacturing phase of MWCNT NMC batteries used inventories generated by the process-based cost model as input for environmental analysis. Although, a profile for MWCNTs was investigated in SimaPro™, the toxicological effects are not represented in LCA results.

The environmental impact assessment results indicate that MWCNT lithium-ion batteries with NMC cathodes created slightly higher environmental burdens in all environmental impact categories compared with conventional NMC batteries due to inclusion of MWCNTs in the process. Because the major input resource and cost in battery manufacturing (with or without CNTs) is energy, an environmental impact assessment to compare the manufacture of MWCNT NMC batteries and traditional NMC batteries was investigated by considering different sources of energy, e.g., US grid with different mixes of solar renewable energy during NMC battery manufacture (100 % US grid, mixing of US grid and 15% solar energy, mixing of US grid and 30% solar energy, and 100% solar energy).

The Cumulative Energy Demand (CED) result indicated that the amount of energy use during battery manufacture remains the same, but the total embodied energy of the battery decreases considerably. For computer batteries manufactured with high EHS levels, energy use is reduced by 280 Kwh and 450 KWh per battery with 15% and 30% solar energy, respectively, compared with energy based 100% on the US grid.

The environmental impact assessment results showed a significant decrease for all environmental impact categories when renewable solar energy is used e.g., 30% solar energy decreases the global warming, ecotoxicity, and ozone depletion by 25%, 22%, and 15%, respectively, during manufacture of one MWCNT NMC battery, compared using

100% US grid. If 100% solar energy were possible, a dramatic reduction of the environmental impacts during battery manufacturing would result compared with base case scenario (100% US grid). Global warming, acidification, and respiratory effects are the environmental impact categories which decrease the most. On the other hand, use of 100% solar energy increases the manufacturing unit cost by approximately $20 for different EHS alternatives compared using 100% US grid.

The PBCM model was used with the output obtained through LCA for manufacture of MWCNTs NMC batteries to develop a complete economic, environmental, health and safety tradeoff analysis. Multi-criteria decision analysis methodology (MCDA) was applied to prioritize the alternatives (batteries with different manufacturing safety standard levels) for decision makers (manufacturers, consumers, regulators, and environmental group analysts) considering their perspectives. As a MCDA methodology, Analytical Hierarchy Process (AHP) technique was used to select the best alternative technology for each stakeholder. As a test case for use of this methodology, preferences were assumed for all decision makers interests. Based on these assumed preferences, results indicate that the most desirable preference for the manufacturers and consumers is to produce MWCNT NMC batteries with high EHS safety levels. The least preferred option for the manufacturers and consumers is to focus on producing the NMC batteries with no CNTs. In comparison, the most desirable option for environmental analysts and regulators is production of NMC batteries with no CNTs followed by CNT NMC batteries with high EHS levels.

Using these methodologies, concurrent assessment of the economic and the environmental health and safety tradeoffs for manufacturing scale-up was explored for the next generation of lithium-ion batteries (MWCNT NMC batteries). The results not only allow consideration of strategies to reduce the manufacturing costs and to utilize sustainable manufacturing practices, but also help manufacturers to estimate the economic viability associated with alternative processing methods to avoid worker exposures during the manufacturing processes.

6.2. Future Work

There are a couple of areas for expanding this work. In this study, the economic and the environmental analysis of manufacturing phase of MWCNT NMC batteries were investigated. In future work, life cycle assessment methodology could be expanded to explore the environmental and human health impacts of MWCNT NMC batteries during their entire life cycle. The toxicological effects of MWCNTs could be also represented in future work. In addition, in end of life phase, if the use of secondary or recycled materials to manufacture the batteries is preferred, the model could be updated to consider the cost drivers of producing recycling materials and disposing the wastes during the recycling process (Figure 6.1). Also, the model could be also expanded to consider the cost of different levels of product stewardship to allow responsible disposal of MWC NMC batteries.

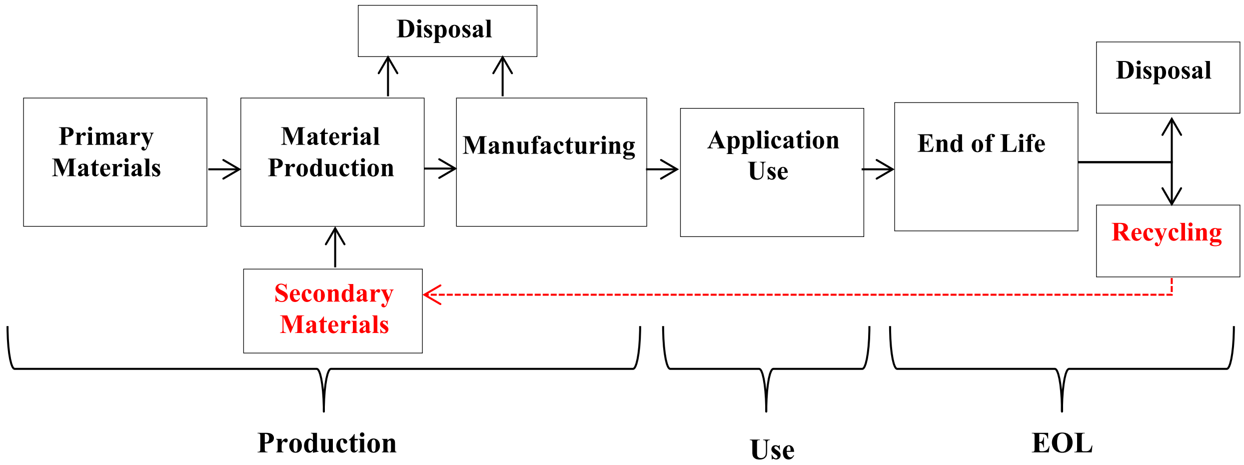


Figure 6-1 Proposed using the secondary materials during battery life cycle

To achieve sustainable manufacturing, battery manufacturing by considering different energy combinations, e.g., US grid with different mixes of solar renewable energy were investigated in this study. It was assumed that the company preferred to purchase an off-site plant renewable energy in order to reduce the environmental burdens. As a future work, the model could be expanded to consider producing on-site renewable energy (installing solar panels) during manufacturing of MWCNT NMC batteries instead of purchasing off-site plant renewable energy. Furthermore, the model could be updated to consider other types of renewable energy such as wind power and found the best combination of US grid and renewable energy (solar or wind power) while considering economic efficiency of MWCNT NMC battery manufacturing.

REFERENCES

Aasgeir Helland, P. W., Andreas Koehler, Kaspar Schmid, and Claudia Som1 (2007). "Reviewing the Environmental and Human Health Knowledge Base

of Carbon Nanotubes." Environmental Health Perspectives 115(8): 7.

Environmental Protection Agency (1993). Life Cycle Assessment: Inventory Guidelines and Principles. O. o. R. a. Development. Cincinnati, Ohio.

Environmental Protection Agency (2006). EPA TSCA Toxic Substances Control Act. 15USC260: 1356-1358.

Environmental Protection Agency (2006). Life Cycle Assessment: Principles and Practice. O. o. R. a. Development. Cincinnati, Ohio, Environmental Protection Agency (EPA) and Scientific Applications International Corporation (SAIC).

Environmental Protection Agency (2007). Nanotechnology White Paper. Washington, EPA: 136.

Environmental Protection Agency (2011). Summary of the Toxic Substances Control Act.

Environmental Protection Agency (2011). "Summery of the Toxic Substances Control Act." from http://www.epa.gov/lawsregs/laws/tsca.html.

Environmental Protection Agency (October 31, 2008). Federal Register Notice: Toxic Substances Control Act Inventory Status of Carbon Nanotubes.

Environmental Protection Agency (2008). TSCA Inventory Status of Nanoscale Substances – General Approach, U.S.

Amarakoon, S., Smith, J., and Segal, B (2013). Aplication of Life Cycle Assessment to Nanoscale technology: Lithium-ion Batteries for Electric Vehicles, Environmental Protection Agency: 1-139.

Antti, V. and S. Justin (2012). "Lithium ion battery production." J Chem Thermodyn 46: 80-85.

Armand, M. and J.-M. Tarascon (2008). "Building better batteries." Nature 451(7179): 652-657.

Ates, M. N., Q. Jia, A. Shah, A. Busnaina, S. Mukerjee and K. M. Abraham (2014). "Mitigation of Layered to Spinel Conversion of a Li-Rich Layered Metal Oxide Cathode Material for Li-Ion Batteries." Journal of The Electrochemical Society 161(3): A290-A301.

Ates, M. N., S. Mukerjee and K. M. Abraham (2014). "A Li-Rich Layered Cathode Material with Enhanced Structural Stability and Rate Capability for Li-on Batteries." Journal of The Electrochemical Society 161(3): A355-A363.

Aurbach, D., Y. Talyosef, B. Markovsky, E. Markevich, E. Zinigrad, L. Asraf, J. S. Gnanaraj and H.-J. Kim (2004). "Design of electrolyte solutions for Li and Li-ion batteries: a review." Electrochimica Acta 50(2): 247-254.

B. Ketterer, U. K., D. Möst, and S. Ulrich (2009). "Lithium-Ion Batteries: State of the Art and Application Potential in Hybrid-, Plug-In Hybrid- and Electric Vehicles,. Karlsruhe, Forschungszentrum Karlsruhe.

Baughman, R. H., Zakhidov, A. A. and de Heer, W. A. (2002). "Carbon Nanotubes--the Route Toward Applications." Science 297(5582): 787-792.

Baumann, H. and A.-M. Tillman (2004). The Hitch Hiker's Guide to LCA. An orientation in life cycle assessment methodology and application, External organization.

Beccali, M., M. Cellura and M. Mistretta (2003). "Decision-making in energy planning. Application of the Electre method at regional level for the diffusion of renewable energy technology." Renewable Energy 28(13): 2063-2087.

Bo Weidema , R. H. (2010). Ecoinvent data v2.2, Swiss Centre for Life Cycle Inventories

Brodd, R. J. and C. Helou (2013). "Cost comparison of producing high-performance Li-ion batteries in the U.S. and in China." Journal of Power Sources 231(0): 293-300.

Buchman, I. (2013). "Battery University." from http://batteryuniversity.com.

Burns, J., A. Kassam, N. Sinha, L. Downie, L. Solnickova, B. Way and J. Dahn (2013). "Predicting and Extending the Lifetime of Li-Ion Batteries." Journal of The Electrochemical Society 160(9): A1451-A1456.

C. Mikolajczak, M. K., K. White, and R. T. Long (2011). Lithium-Ion Batteries Hazard and Use Assessment,, Fire Protection Research Foundation, Quincy, Massachusetts,.

Caitlin Fisher, A. E. R., Zhao Jun Han, (2012). "Applications and Nanotoxicity of Carbon Nanotubes and Graphene in Biomedicine." Journal of Nanomaterials 2012: 19.

Carrascosa, L. G., M. Moreno, M. Álvarez and L. M. Lechuga (2006). "Nanomechanical biosensors: a new sensing tool." TrAC Trends in Analytical Chemistry 25(3): 196-206.

Chan, C. K., H. Peng, G. Liu, K. McIlwrath, X. F. Zhang, R. A. Huggins and Y. Cui (2008). "High-performance lithium battery anodes using silicon nanowires." Nature nanotechnology 3(1): 31-35.

Che, J., T. Cagin and W. A. Goddard III (2000). "Thermal conductivity of carbon nanotubes." Nanotechnology 11(2): 65.

ChemPages. (2012). "lectrochemistry: Primary and Secondary Batteries." from http://www.chem.wisc.edu/deptfiles/genchem/netorial/ROttosen/tutorial/modules/electrochemistry/06battery/18_61.htm.

Chen, S., C. Mi, L. Su, B. Gao, Q. Fu and X. Zhang (2009). "Improved performances of mechanical-activated LiMn2O4/MWNTs cathode for aqueous rechargeable lithium batteries." Journal of Applied Electrochemistry 39(10): 1943-1948.

Cheng, F., J. Liang, Z. Tao and J. Chen (2011). "Functional Materials for Rechargeable Batteries." Advanced Materials 23(15): 1695-1715.

Chong, J., S. Xun, H. Zheng, X. Song, G. Liu, P. Ridgway, J. Q. Wang and V. S. Battaglia (2011). "A comparative study of polyacrylic acid and poly (vinylidene difluoride) binders for spherical natural graphite/LiFePO 4 electrodes and cells." Journal of Power Sources 196(18): 7707-7714.

United Nation Global Compact (2009). Global Sustainability in the 21st Century. An Action Plan for Business.

PRé Consultants (2011). "SimaPro 7.3.3." from http://www.pre-sustainability.com/simapro-lca-software.

Roland Berger Strategy Consultants (2013). "Lithium-ion battery Global Market Size." from http://www.rolandberger.us/media/pdf/Roland_Berger_ta_Size_Matters_20130114.pdf.

National Science and Technology Council (2014). Supplement to the President's Budget for Fiscal Year 2015, The National Nanotechnology Initiative.

De Andrade, J., P. R. Impinnisi and D. L. Do Vale (2011). "180 Ah kg(-1) specific capacity positive tubular electrodes for lead acid batteries." Journal of Power Sources 196(10): 4832-4836.

de las Casas, C. and W. Li (2012). "A review of application of carbon nanotubes for lithium ion battery anode material." Journal of Power Sources 208: 74-85.

Dresselhaus, A. J. a. M. (2008). Carbon Nanotubes: Advanced Topics in the Synthesis, Structure, Properties, and Applications, Springer.

Dresselhaus, M. S., G. Dresselhaus, J. C. Charlier and E. Hernández (2004). "Electronic, thermal and mechanical properties of carbon nanotubes." Philosophical Transactions of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences 362(1823): 2065-2098.

Dunens, O. M., K. J. MacKenzie and A. T. Harris (2010). "Large-Scale Synthesis of Double-Walled Carbon Nanotubes in Fluidized Beds." Industrial & Engineering Chemistry Research 49(9): 4031-4035.

El-Ansary, A. and S. Al-Daihan (2009). "On the Toxicity of Therapeutically Used Nanoparticles: An Overview." Journal of Toxicology 2009.

Espinoza, V. S., S. Erbis, L. Pourzahedi, M. J. Eckelman and J. A. Isaacs (2014). "Material Flow Analysis of Carbon Nanotube Lithium-Ion Batteries Used in Portable Computers." ACS Sustainable Chemistry & Engineering 2(7): 1642-1648.

Etacheri, V., R. Marom, R. Elazari, G. Salitra and D. Aurbach (2011). "Challenges in the development of advanced Li-ion batteries: a review." Energy & Environmental Science 4(9): 3243-3262.

Fadri Gottschalk, B. N., Bernd Gawlik (2010). Report on Exposure Scenarios and Release of Nanomaterials to the Environment. St. Gallen, Swiss Federal Laboratories for Materials Science and Technology.

Fadri Gottschalk, B. N., Bernd Gawlik (2010). Report on Exposure Scenarios and Release of Nanomaterials to the Environment 1-93.

Frischknecht, R. and K. Flury (2011). "Life cycle assessment of electric mobility: answers and challenges—Zurich, April 6, 2011." The International Journal of Life Cycle Assessment 16(7): 691-695.

Frischknecht, R., N. Jungbluth, H.-J. Althaus, R. Hischier, G. Doka, C. Bauer, R. Dones, T. Nemecek, S. Hellweg and S. Humbert (2007). Implementation of life cycle impact assessment methods. Data v2. 0 (2007). Ecoinvent report No. 3, Ecoinvent Centre, Swiss Federal Laboratories for Materials Testing and Research (EMPA), Duebendorf (Switzerland).

Fuchs, E. R. H., E. J. Bruce, R. J. Ram and R. E. Kirchain (2006). "Process-based cost modeling of photonics manufacture: the cost competitiveness of monolithic integration of a 1550-nm DFB laser and an electroabsorptive modulator on an InP platform." Lightwave Technology, Journal of 24(8): 3175-3186.

Gagliardi, M. (2014). Global Markets and Technologies for Nanofiltration, BCC Research.

Sullivan J.L. and L. Gaines (2010). A Review of Battery Life-Cycle Analysis: State of Knowledge and Critical Needs, US Department of Energy.

Goodenough, J. B. (2012). "Evolution of Strategies for Modern Rechargeable Batteries." Accounts of Chemical Research.

Gottesfeld, P. and A. K. Pokhrel (2011). "Review: Lead Exposure in Battery Manufacturing and Recycling in Developing Countries and Among Children in Nearby Communities." Journal of Occupational and Environmental Hygiene 8(9): 520-532.

Han, Z. J., S. Yick, I. Levchenko, E. Tam, M. M. A. Yajadda, S. Kumar, P. J. Martin, S. Furman and K. Ostrikov (2011). "Controlled synthesis of a large fraction of metallic single-walled carbon nanotube and semiconducting carbon nanowire networks." Nanoscale 3(8): 3214-3220.

Hankin, S. (2010). Lithium-Ion Batteries and Carbon Nanotubes. Safenano, Europe's Center of Excellence Nanotechnology Hazard and Risk.

Hartmann II, R. L. (2008). An aging model for lithium-ion cells, The University of Akron.

National Institute for Occupational Safety and Health (2011). Occupational Exposure to Carbon Nanotubes and Nanofibers.

Hischier, R. and T. Walser (2012). "Life cycle assessment of engineered nanomaterials: State of the art and strategies to overcome existing gaps." Science of The Total Environment 425(0): 271-282.

Hsieh, S.-F., D. Bello, D. F. Schmidt, A. K. Pal and E. J. Rogers (2012). "Biological oxidative damage by carbon nanotubes: Fingerprint or footprint?" Nanotoxicology 6(1): 61-76.

Huang, K., J. Li and Z. Xu (2010). "Characterization and recycling of cadmium from waste nickel–cadmium batteries." Waste Management 30(11): 2292-2298.

Ibtisam E, T. (2009). "Biosensors for cancer markers diagnosis." Seminars in Cell & Developmental Biology 20(1): 55-62.

Panasonic Inc (2014). "Lithium Ion UF553436G." from http://na.industrial.panasonic.com/sites/default/pidsa/files/uf553436g_0.pdf.

Siemens Inc (2014). "Battery Manufacturing Process." from http://www.industry.siemens.com/topics/global/en/batterymanufacturing/process/pages/default.aspx.

Yardney Technical Products Inc (2014). from http://yardney.com/.

National Nanotechnology Initiative (2007). "Prioritization of environmental, health, and safety research needs for engineerednanoscale materials: An interim document for public comment, National Nanotechnology

National Nanotechnology Initiative, National Science and Technology Council.", from www.nano.gov/Prioritization_EHS_Research_Needs_Engineered_Nanoscale_Materials.pdf. Accessed February 2009.

National Nanotechnology Initiative (2008). "Strategy for nanotechnology-related environmental, health, and safety research

National Nanotechnology Initiative, National Science and Technology Council.", from http://www.nano.gov/NNI_EHS_Research_Strategy.pdf. Accesses March 2010.

National Nanotechnology Initiative (2013). "Nanotechnology Benefits and Applications."

Isaacs, J., Tanwani, A., Healy, ML., Dahlben, LJ (2010). "Economic assessment of single-walled carbon nanotube processes." Journal of Nanoparticle Research 12(2): 551-562.

Isaacs, J. A., A. Tanwani, M. L. Healy and L. J. Dahlben (2010). "Economic assessment of single-walled carbon nanotube processes." Journal of Nanoparticle Research 12(2): 551-562.

Ishikawa, M., T. Sugimoto, M. Kikuta, E. Ishiko and M. Kono (2006). "Pure ionic liquid electrolytes compatible with a graphitized carbon negative electrode in rechargeable lithium-ion batteries." Journal of power sources 162(1): 658-662.

Jianrong, C., M. Yuqing, H. Nongyue, W. Xiaohua and L. Sijiao (2004). "Nanotechnology and biosensors." Biotechnology Advances 22(7): 505-518.

Jin, B., H.-B. Gu, W. Zhang, K.-H. Park and G. Sun (2008). "Effect of different carbon conductive additives on electrochemical properties of LiFePO4-C/Li batteries." Journal of Solid State Electrochemistry 12(12): 1549-1554.

Johnson, M. and R. Kirchain (2009). "Quantifying the effects of parts consolidation and development costs on material selection decisions: A process-based costing approach." International Journal of Production Economics 119(1): 174-186.

Johnson, M. D. and R. Kirchain (2010). "Developing and Assessing Commonality Metrics for Product Families: A Process-Based Cost-Modeling Approach." Engineering Management, IEEE Transactions on 57(4): 634-648.

Joho, F., B. Rykart, A. Blome, P. Novák, H. Wilhelm and M. E. Spahr (2001). "Relation between surface properties, pore structure and first-cycle charge loss of graphite as negative electrode in lithium-ion batteries." Journal of Power Sources 97–98(0): 78-82.

Kablan, M. (2004). "Decision support for energy conservation promotion:: an analytic hierarchy process approach." Energy policy 32(10): 1151-1158.

Kathy Hart, M. A. C., and Clive Davies (2012). Lithium-ion Batteries and Nanotechnology for Electric Vehicles, Environmental Protection Agency.

Kim, T. H., I. K. Park, J. W. Nah, Y. J. Choi and C. S. Cho (2004). "Galactosylated chitosan/DNA nanoparticles prepared using water-soluble chitosan as a gene carrier." Biomaterials 25(17): 3783-3792.

Ko, S., J. I. Lee, H. S. Yang, S. Park and U. Jeong (2012). "Mesoporous CuO Particles Threaded with CNTs for High-Performance Lithium-Ion Battery Anodes." Advanced Materials 24(32): 4451-4456.

Kozarsky, R. (2014). "Searching for Profits at the Intersection of Nanotech and Electronics.", from http://sites.ieee.org/sfbanano/files/2013/12/Lux_Research-Ross_Kozarsky-IEEE_Nano_2014-01-28.pdf.

Kubis, R. (2012). "Eurobat." from http://www.eurobat.org/battery-technologies.

Kularatna, N. (2011). "Rechargeable batteries and their management." Instrumentation & Measurement Magazine, IEEE 14(2): 20-33.

Landi, B. J., M. J. Ganter, C. D. Cress, R. A. DiLeo and R. P. Raffaelle (2009). "Carbon nanotubes for lithium ion batteries." Energy & Environmental Science 2(6): 638-654.

Lasjaunias, J.-C. (2003). "Thermal properties of carbon nanotubes." Comptes Rendus Physique 4(9): 1047-1054.

Lee, J., S. Mahendra and P. J. J. Alvarez (2010). "Nanomaterials in the Construction Industry: A Review of Their Applications and Environmental Health and Safety Considerations." ACS Nano 4(7): 3580-3590.

Leonard, M. P. A. a. F. (2007). Physics of carbon nanotube electronic devices. Center for Nanotechnology, NASA Ames Research Center,.

Leuenberger, M. and R. Frischknecht (2010). "Life cycle assessment of battery electric vehicles and concept cars." Report, ESU-Services Ltd.

Lewandowski, A. and A. Świderska-Mocek (2009). "Ionic liquids as electrolytes for Li-ion batteries—an overview of electrochemical studies." Journal of Power Sources 194(2): 601-609.

Li, Y., Y. Wei, G. Shi, Y. Xian and L. Jin (2011). "Facile Synthesis of Leaf-Like CuO Nanoparticles and Their Application on Glucose Biosensor." Electroanalysis 23(2): 497-502.

Lindsay J. Dahlben, J. A. I. (2009). Environmental Assessment of Manufacturing with Carbon Nanotubes. The International Symposium on Sustainable Systems and Technology: 5.

Lindsay J. Dahlben, J. A. I. (2010). Investigation of the Environmental Implications of the CNT Switch through its Life Cycle. Master of Science, Northeatern University.

Locascio, A. (2000). "Manufacturing Cost Modeling for Product Design." International Journal of Flexible Manufacturing Systems 12(2-3): 207-217.

Celina M; M. Kahn; K.White; T. Long (2011). Lithium-ion Batteries Hazard and Use Assessment, Springer US.

Maes, H., A. Schaeffer, H. Hollert and H. Ratte (2009). "Nanomaterials: risks and benefits (Editors: Igor Linkov & Jeffery Steevens)." Environmental Science and Pollution Research 16(6): 741-742.

Majeau-Bettez, G., T. R. Hawkins and A. H. Strømman (2011). "Life Cycle Environmental Assessment of Lithium-Ion and Nickel Metal Hydride Batteries for Plug-In Hybrid and Battery Electric Vehicles." Environmental Science & Technology 45(10): 4548-4554.

Marks, T., S. Trussler, A. Smith, D. Xiong and J. Dahn (2011). "A guide to Li-ion coin-cell electrode making for academic researchers." Journal of The Electrochemical Society 158(1): A51-A57.

Marry Ann Curran (2006). Life Cycle Assessment: Principles and practice. Reston, Environmental Protection Agency.

Meagan L. Healy, L. J. D., and Jacqueline A. Isaacs (2008). "Environmental Assessment of Single-Walled Carbon Nanotube Processes." Journal of Industrial Ecology 12(3): 376-396.

Musee, N. (2011). "Nanowastes and the environment: Potential new waste management paradigm." Environment International 37(1): 112-128.

Nadeau, M.-C., A. Kar, R. Roth and R. Kirchain (2010). "A dynamic process-based cost modeling approach to understand learning effects in manufacturing." International Journal of Production Economics 128(1): 223-234.

Nanowerk. (2011). "Global Carbon Nanotubes Market Outlook: Industry Beckons." from http://www.ckmnt.com/Global%20carbon%20nanotubes%20market%20-%20industry%20beckons.pdf.

National Institute for Occupational Safety and Health (2010). Current Intelligence Bulletin Occupational Exposure to Carbon Nanotubes and Nanofibers;.

National Institute for Occupational Safety and Health (2013). Occupational Exposure to Carbon Nanotubes and Nanofibers;. Current Intelligence Bulletin 65: 1-145.

Notter, D. A., M. Gauch, R. Widmer, P. Wäger, A. Stamp, R. Zah and H.-J. Althaus (2010). "Contribution of Li-Ion Batteries to the Environmental Impact of Electric Vehicles." Environmental Science & Technology 44(17): 6550-6556.

Notter, D. A., M. Gauch, R. Widmer, P. Wager, A. Stamp, R. Zah and H.-J. r. Althaus (2010). "Contribution of Li-ion batteries to the environmental impact of electric vehicles." Environmental science & technology 44(17): 6550-6556.

Olapiriyakul, S. (2010). End-of-Life Analysis of Nanotechnology Products. Doctoral of Philosophy in Industrial Engineering, New Jersey's Science & Technology University.

International Organization for Standardization (2006). Environmental Management-Life Cycle Assessment-Principals and Framework. ISO 14040. Switzerland, International Organization for Standardization.

International Standards Organization (2006). Environmental Management-Life Cycle Assessment-Principals and Framework.

World Health Organization (2011). Guidelines on quality risk management: 1-260.

Nelson, P., K. G. G., I. Bloom, D.W. Dees (2011). Modeling the Performance and Cost of Lithium-Ion Batteries for Electric-Drive Vehicles, Argonne National Laboratory: 121.

Paresh Chandra Ray, H. Y., Peter P. Fu (2009). "Toxicity and Environmental Risks of Nanomaterials: Challenges and Future Needs." Environmental Science and Health Part 27(1): 36.

Peng, K., Y. Yan, S. Gao and J. Zhu (2003). "Dendrite-Assisted Growth of Silicon Nanowires in Electroless Metal Deposition." Advanced Functional Materials 13(2): 127-132.

United Nations Environment Programme (2011). Towards a green economy: pathways to sustainable development and poverty eradication.

Ramadass, P., B. Haran, R. White and B. N. Popov (2003). "Mathematical modeling of the capacity fade of Li-ion cells." Journal of Power Sources 123(2): 230-240.

Research, G. V. (2012). "Microscopes Market Analysis By Product, y Application, and Segment Forecasts ", from http://www.grandviewresearch.com/industry-analysis/microscopes-industry.

Rosenbaum, R. K., T. M. Bachmann, L. S. Gold, M. A. Huijbregts, O. Jolliet, R. Juraske, A. Koehler, H. F. Larsen, M. MacLeod and M. Margni (2008). "USEtox—the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment." The International Journal of Life Cycle Assessment 13(7): 532-546.

Rydh, C. J. and M. Karlström (2002). "Life cycle inventory of recycling portable nickel–cadmium batteries." Resources, Conservation and Recycling 34(4): 289-309.

Saaty, T. L. (2008). "Decision making with the analytic hierarchy process." International journal of services sciences 1(1): 83-98.

Samaras, C. and K. Meisterling (2008). "Life cycle assessment of greenhouse gas emissions from plug-in hybrid vehicles: implications for policy." Environmental science & technology 42(9): 3170-3176.

Sankey, P., D. T. Clark and S. Micheloto (2010). "The End of the Oil Age, 2011 and beyond: a reality check." Deutsche Bank 22.

Scrosati, B. and J. Garche (2010). "Lithium batteries: Status, prospects and future." Journal of Power Sources 195(9): 2419-2430.

Shah, A., M. N. Ates, S. Kotz, J. Seo, K. M. Abraham, S. Somu and A. Busnaina (2014). "A Layered Carbon Nanotube Architecture for High Power Lithium Ion Batteries." Journal of The Electrochemical Society 161(6): A989-A995.

Shanika Amarakoon, J. S., and Brian Segal (2013). Lithium-ion Batteriesand Nanotechnology for Electric Vehicles: A Life Cycle Assessment, Environmental Protection Agency 1-123.

Sharifi, S., S. Behzadi, S. Laurent, M. Laird Forrest, P. Stroeve and M. Mahmoudi (2012). "Toxicity of nanomaterials." Chemical Society Reviews 41(6): 2323-2343.

Shim, J. and K. A. Striebel (2003). "Cycling performance of low-cost lithium ion batteries with natural graphite and LiFePO 4." Journal of Power Sources 119: 955-958.

Shvedova, A. A., E. Kisin, et al. (2008). (2008). "Inhalation vs. aspiration of single-walled carbon nanotubes in C57BL/6 mice: inflammation, fibrosis, oxidative stress, and mutagenesis." Am J Physiol Lung Cell Mol Physiol 295(4): 552-565.

Siavoshi, S., C. Yilmaz, S. Somu, T. Musacchio, J. R. Upponi, V. P. Torchilin and A. Busnaina (2011). "Size-Selective Template-Assisted Electrophoretic Assembly of Nanoparticles for Biosensing Applications." Langmuir 27(11): 7301-7306.

Sipahi, S. and M. Timor (2010). "The analytic hierarchy process and analytic network process: an overview of applications." Management Decision 48(5): 775-808.

Smith, A., J. Burns and J. Dahn (2010). "A high precision study of the Coulombic efficiency of Li-ion batteries." Electrochemical and Solid-State Letters 13(12): A177-A179.

Snyders, C., E. E. Ferg and T. van Dyl (2012). "The use of a Polymat material to reduce the effects of sulphation damage occurring in negative electrodes due to the partial state of charge capacity cycling of lead acid batteries." Journal of Power Sources 200: 102-107.

Song, M.-K., S. Park, F. M. Alamgir, J. Cho and M. Liu (2011). "Nanostructured electrodes for lithium-ion and lithium-air batteries: the latest developments, challenges, and perspectives" Materials Science and Engineering: R: Reports 72(11): 203-252.

Stamp, A., D. J. Lang and P. A. Wäger (2012). "Environmental impacts of a transition toward e-mobility: the present and future role of lithium carbonate production." Journal of Cleaner Production 23(1): 104-112.

International Organization for Standardization (2006). "ISO 14040:2006."

Stander, L. and L. Theodore (2011). "Environmental Implications of Nanotechnology—An Update." International Journal of Environmental Research and Public Health 8(2): 470-479.

Stander, L. a. T., L. (2011). "Environmental Implications of Nanotechnology—An Update." International Journal of Environmental Research and Public Health 8: 470-479.

Steele, N. L. and D. T. Allen (1998). "Peer Reviewed: An Abridged Life-Cycle Assessment of Electric Vehicle Batteries." Environmental science & technology 32(1): 40A-46A.

Sullivan, J. L. and L. Gaines (2012). "Status of life cycle inventories for batteries." Energy Conversion and Management 58: 134-148.

Teow, Y., P. V. Asharani, M. P. Hande and S. Valiyaveettil (2011). "Health impact and safety of engineered nanomaterials." Chemical Communications 47(25): 7025-7038.

Thackeray, M. M., C. Wolverton and E. D. Isaacs (2012). "Electrical energy storage for transportation—approaching the limits of, and going beyond, lithium-ion batteries." Energy & Environmental Science 5(7): 7854-7863.

Trahey, L., C. Johnson, J. Vaughey, S.-H. Kang, L. Hardwick, S. Freunberger, P. Bruce and M. Thackeray (2011). "Activated lithium-metal-oxides as catalytic electrodes for Li–O2 cells." Electrochemical and Solid-State Letters 14(5): A64-A66.

Tudela, A., N. Akiki and R. Cisternas (2006). "Comparing the output of cost benefit and multi-criteria analysis: An application to urban transport investments." Transportation Research Part A: Policy and Practice 40(5): 414-423.

Georgia State University (2012). "Standard Electrode Potentials in Aqueous Solution." from http://hyperphysics.phy-astr.gsu.edu/hbase/tables/electpot.html.

Vaddiraju, S., I. Tomazos, D. J. Burgess, F. C. Jain and F. Papadimitrakopoulos (2010). "Emerging synergy between nanotechnology and implantable biosensors: A review." Biosensors and Bioelectronics 25(7): 1553-1565.

Venkata Upadhyayula, D. M., Marry Ann Curran, Michael Gonzalez (2011). "Measuring the Environmental Performance of Carbon Nanotube Enabled Nanoproducts Using Life Cycle Assessment." Journal of Cleaner Production: 1-35.

Vinayan, B., R. Nagar, V. Raman, N. Rajalakshmi, K. Dhathathreyan and S. Ramaprabhu (2012). "Synthesis of graphene-multiwalled carbon nanotubes hybrid nanostructure by strengthened electrostatic interaction and its lithium ion battery application." Journal of Materials Chemistry 22(19): 9949-9956.

Wang, J.-J., Y.-Y. Jing, C.-F. Zhang and J.-H. Zhao (2009). "Review on multi-criteria decision analysis aid in sustainable energy decision-making." Renewable and Sustainable Energy Reviews 13(9): 2263-2278.

Wang, J., P. Liu, J. Hicks-Garner, E. Sherman, S. Soukiazian, M. Verbrugge, H. Tataria, J. Musser and P. Finamore (2011). "Cycle-life model for graphite-LiFePO4 cells." Journal of Power Sources 196(8): 3942-3948.

Wang, Y., J. Travas-Sejdic and R. Steiner (2002). "Polymer gel electrolyte supported with microporous polyolefin membranes for lithium ion polymer battery." Solid State Ionics 148(3): 443-449.

Wen-Tso, L. (2006). "Nanoparticles and their biological and environmental applications." Journal of Bioscience and Bioengineering 102(1): 1-7.

Wen-Tso, L. (2007). "Nanoparticles and their biological and environmental applications." Journal of Bioscience and Bioengineering 102: 1-7.

Wu, H., G. Chan, J. W. Choi, Y. Yao, M. T. McDowell, S. W. Lee, A. Jackson, Y. Yang, L. Hu and Y. Cui (2012). "Stable cycling of double-walled silicon nanotube battery anodes through solid-electrolyte interphase control." Nature nanotechnology 7(5): 310-315.

Xu, J., G. Chen and X. Li (2009). "Electrochemical performance of LiFePO4 cathode material coated with multi-wall carbon nanotubes." Materials Chemistry and Physics 118(1): 9-11.

Xu, K. (2004). "Nonaqueous liquid electrolytes for lithium-based rechargeable batteries." Chemical reviews 104(10): 4303-4418.

Yoshino, A. (2012). "The Birth of the Lithium-Ion Battery." Angewandte Chemie International Edition 51(24): 5798-5800.

Zackrisson, M., L. Avellán and J. Orlenius (2010). "Life cycle assessment of lithium-ion batteries for plug-in hybrid electric vehicles–Critical issues." Journal of Cleaner Production 18(15): 1519-1529.

Zackrisson, M., L. Avellán and J. Orlenius (2010). "Life cycle assessment of lithium-ion batteries for plug-in hybrid electric vehicles – Critical issues." Journal of Cleaner Production 18(15): 1519-1529.

Zaghib, K., M. Dontigny, A. Guerfi, P. Charest, I. Rodrigues, A. Mauger and C. Julien (2011). "Safe and fast-charging Li-ion battery with long shelf life for power applications." Journal of Power Sources 196(8): 3949-3954.

Zang, J.-L. and Y.-P. Zhao (2012). "Silicon nanowire reinforced by single-walled carbon nanotube and its applications to anti-pulverization electrode in lithium ion battery." Composites Part B: Engineering 43(1): 76-82.

Zhang, G. Y., X. W. Zhao, J. X. Qiang, F. Tian and L. Yang (2012). "New lead-acid battery management system based on generator regulation." International Journal of Automotive Technology 13(4): 679-686.

Zhang, H., G. Cao, Z. Wang, Y. Yang, Z. Shi and Z. Gu (2010). "Carbon nanotube array anodes for high-rate Li-ion batteries." Electrochimica Acta 55(8): 2873-2877.

Zhang, S. S. (2007). "A review on the separators of liquid electrolyte Li-ion batteries." Journal of Power Sources 164(1): 351-364.

Zhang, W.-J. (2011). "Structure and performance of LiFePO4 cathode materials: A review." Journal of Power Sources 196(6): 2962-2970.

Zheng, B., S. Xie, L. Qian, H. Yuan, D. Xiao and M. M. F. Choi (2011). "Gold nanoparticles-coated eggshell membrane with immobilized glucose oxidase for fabrication of glucose biosensor." Sensors and Actuators B: Chemical 152(1): 49-55.

Zheng, H., J. Li, X. Song, G. Liu and V. S. Battaglia (2012). "A comprehensive understanding of electrode thickness effects on the electrochemical performances of Li-ion battery cathodes." Electrochimica Acta 71: 258-265.

Zhou, C., K. Qian, M. Allan and W. Zhou (2011). "Modeling of the cost of EV battery wear due to V2G application in power systems." Energy Conversion, IEEE Transactions on 26(4): 1041-1050.

Zimmermann, B. (2012). Integration of carbon nanotubes in lithium-ion traction batteries from an environmental perspectiveUniversity of Applied Sciences Munich.

Zopounidis, C. and M. Doumpos (2013). "Multicriteria decision systems for financial problems." Top 21(2): 241-261.

Zopounidis, C. and P. Pardalos (2010). Handbook of multicriteria analysis, Springer Science & Business Media.

APPENDIX

MWCNT Inventory database for SimaPro™

Inputs		Outputs	
Material inputs		**Emission outputs**	
CO	3,471.00kg/h		
Co	19.00kg/h	Co2O3	26.00kg/h
Mo	19.00kg/h	MoO3	28.00kg/h
SiO2	1.30kg/h	SiO2	1.30kg/h
O2	9.00kg/h		
H2O	714.87kg/h	H2O	228.80kg/h
NaOH 50% solution	36.48kg/h	NaOH 50% solution	32.20kg/h
HCl 100%	3.90kg/h	NaCl	6.25kg/h
MEA	8.54kg/h	MEA	8.54kg/h
Ethoxylated alcohol	33.52kg/h		
H2O (cooling)	66,422.00kg/h	H2O (water)	59,089.00kg/h
		H2O (steam)	7,588.00kg/h
		CO2	3,275.35kg/h
		H2	25.00kg/h
		Product outputs	
		MWCNT	595.00kg/h
		CoCl2	0.04kg/h
		MoCl2	0.05kg
Energy inputs		**Energy-use emissions**	
Natural gas	34,560.813MJ/h	Emissions in background system	
Electricity	387kW		
Infrastructure inputs		**Infrastructure outputs**	
Chemical plant	1.19E-6 unit/h	Emissions in background system	
Transport truck, 3.5-16 to (Co, Mo)	19tkm/h		
Transport ship (Mo)	133tkm/h		
Disposal inputs		**Disposal outputs**	
Solvent incineration	8.54kg/h	Emissions in background system	
Inert waste	55.30kg/h		
Sewage plant	0.26m3/h		

Life Cycle Perspectives for Biosensors

Ali Hakimian[1], Pegah N. Abadian[1] and Jacqueline A Isaacs[1]

[1] Department of Mechanical and Industrial Engineering, Northeastern University, Boston MA, USA

Abstract

Innovative nanotechnologies have led to the creation of a wide variety of nanomaterials for use in consumer products, healthcare, electronics, drug delivery, and agriculture. In biomedical applications, biosensors play a crucial role in detection of various diseases, and nanoscale biosensors offer enhanced detection capabilities. LCA methods are used to explore the nanomanufacturing phase of polystyrene latex nanoparticle biosensors. LCI results obtained using SimaPro™ software indicate that within the fabrication stage of the lifecycle for these devices, there are three processes that show greatest contribution to the environmental footprint: photoresist, e-beam lithography, and Au film deposition.

INTRODUCTION

Effective methods for disease diagnosis are important for on-time disease identification and for applying required treatment before drug resistance and additional infections occur. Hence there is a need to develop detection devices that are fast, sensitive, selective, reusable, cheap and easy to use as an alternative to classical time consuming and heavy lab instrumentations (Zheng, Xie et al. 2011). Biosensors are promising devices for fulfilling these needs. The common means to measure the blood sugar level for diabetic patients requires finger pricking. This method does not measure the amount of blood glucose continuously and uses needles each time, which is inconvenient and creates more waste (Li, Wei et al. 2011). Use of biosensors for diagnosis would be a cost effective, fast, and simple alternative to heavy lab instruments. Developments in medical and scientific areas indicate a need for a method to continuously monitor metabolic processes for imbalances in the body, which would help in early disease or disorder detection. Thus the development of implantable biosensors is an area of particular interest. Biosensors have the potential for use as an alternative for current diagnosis methods, such as mass spectroscopy, enzyme linked immunosorbent assays (ELISA), chromatography and glucose test strips (Vaddiraju, Tomazos et al. 2010).

Biosensors are analytical devices which consist of three parts; 1) a recognition element, which in biosensors is a biological recognition element such as an enzyme or antibody, 2) a transducer, which converts the changes in the biorecognition element to a measurable signal, and 3) the processor, which processes the signal received from the transducer. The recognition element is paired with a transducer to translate the bio-recognition event into a measurable effect, such as mechanical motion, an electrical signal or an optical emission (Carrascosa, Moreno et al. 2006). Figure 1 shows a schematic of how a biosensor works.

Improvements in synthesizing nanoscale materials and controlling their properties, have contributed to their use in broad areas of application including advanced materials, electronics, magnetic and optoelectronics, biomedicine, pharmaceuticals, cosmetics, energy, and catalytic and environmental detection and monitoring (Wen-Tso 2006). The nanoscale dimensions (with at least one dimension less that 100 nm and more than atomic/molecular scale) in nanomaterials contribute to their unique physical, chemical and biological characteristics. The distinctive properties of nanomaterials offer the promise of great advances in many scientific and technological areas, including biosensors.

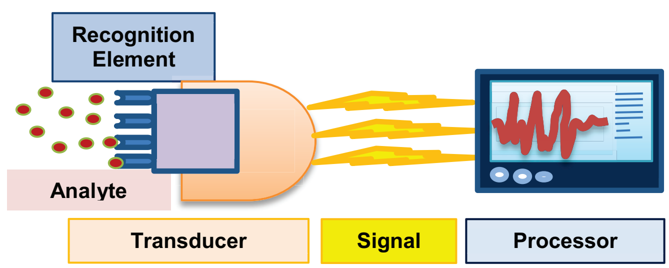


Figure 1: Schematic diagram of a biosensor

In the area of biosensors, nanotechnology is playing very important role. As the size of a material decreases to less than 100 nm, unique characteristics become apparent that differ from the bulk material, such as, marked changes in thermal and optical properties, enhanced reactivity and catalytic activity, faster electron/Ion transport, negative refractivity and novel quantum mechanical properties (Vaddiraju, Tomazos et al. 2010). Researchers categorize the nanoparticles (NPs) that are used in biosensors into four groups: semiconductor NPs, magnetic NPs, metal NPs and other types (including polymeric nanopolymers, silica nanoparticles, etc.). Nanoparticles can be used as the bio-recognition element or the transducer or both. By modifying the surface of NPs with functional groups, these molecules become capable of binding with biological molecules and consequently will improve the detection and amplification of signals in biosensors (Jianrong, Yuqing et al. 2004). The four main characteristics of the biosensors include: i) selectivity, which relates to the ability of the sensor to distinguish between targeted analyte and other components; ii) sensitivity, which is the value of the electrode response per substrate concentration: iii) detection time, which refers to the necessity of having 95% of the response; iv) linearity, which is the maximum linear value of the sensor calibration curve. Linearity of the sensor must be high for detection of high substrate concentration. Various researchers have shown that the use of NPs in biosensors markedly improves the specificity of detection, sensitivity, detection time and linearity (Vaddiraju, Tomazos et al. 2010, Li, Wei et al. 2011, Zheng, Xie et al. 2011), due to the small physical size of the NPs that reduces the activity change of the biological parts. One of the important components of biosensors is the bio-recognition area which interacts with the analyte and influences the sensitivity of the biosensor. Because NPs have high surface to volume ratios, NPs increase the surface area to provide more available sites for molecular interaction and increase the sensitivity of the biosensor. Single molecule detection would be very useful for cancer diagnosis (Kim, Park et al. 2004, Ibtisam E 2009).

2 UNINTENDED CONSEQUENCES OF RELEASES

Release of nanoparticles could potentially occur throughout the entire life cycle of a nano-enabled product, including during the production process, manufacturing, use, and recycling or disposal of the nanoproducts (Olapiriyakul 2010). Nanomaterial releases during production or manufacturing processes could be categorized as direct or indirect. Direct releases to air could occur during transportation or through spills. Indirect releases can happen when treated or untreated wastewater somehow reaches a river or landfill (Paresh Chandra Ray 2009, Fadri Gottschalk 2010, Olapiriyakul 2010). Figure 2 shows potential nanoparticle release scenarios for the life cycle of a nanoproduct.

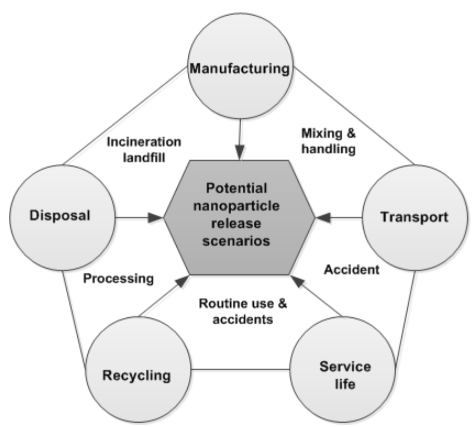


Figure 2: The life cycle and environmental fate of NPs (Hankin 2010).

The level and pattern of releases is highly dependent on how the manufactured nanomaterial is embedded within the product. For instance, manufactured nanomaterials in fluids release very quickly during the use phase, and in most cases complete release happens during the life cycle. However, the release of manufactured nanomaterials embedded in solid matrices would happen gradually with only partial or zero releases during the life cycle (Fadri Gottschalk 2010).

Manufacturing with nanomaterials is still in the early stages, and there are concerns with regard to the environmental health and safety of workers who may be exposed to the nanomaterials. Nanoparticles can pass through the skin or become inhaled, causing lung damage. Though there are no established regulations for safe practices, waste handling and disposal while working with nanomaterials, the National Institute for Occupational Safety and Health (NIOSH) suggests handling NPs with a hazard-based approach. The U.S. Environmental Protection Agency (EPA) is also beginning to list some NPs in the Toxic Substances Control Act inventory. Indeed there are so many uncertainties about products containing nanoparticles in terms of long term impact on the environment, sustainability and end of life management (Agency 2011, Musee 2011, Stander and Theodore 2011).

2 BIOSENSOR FABRICATION USING NANOPARTICLES

The biosensor investigated in this study uses polystyrene latex (PSL) nanoparticles as a base for a functionalized biosensor. The process flow path for the fabrication of the PSL biosensor is shown in Figure 3. The process steps are typical of semiconductor manufacturing. The functional unit for making PSL biosensors is established as a 3" silicon wafer. In the first step, deionized (DI) water is used in large quantities, because wafers need to be cleaned carefully. Then, the wafers are dried by nitrogen. The next step involves chromium deposition, using a magnetron sputter deposition system to deposit 2 nm Cr sacrificial and 50 nm gold (Au) layer. After re-cleaning the wafers with acetone, isopropanol, and deionized water, the wafers are placed in the oven for 2 minutes at 450°C. Photoresist (PMMA) is spun onto the wafer to achieve a controlled thickness. Then, a hot plate is used to bake the wafers. In the first heating cycle, the baking duration is about 4 minutes with a temperature of 65°C. The second heating cycle duration is about 10 minutes at 95°C. Electron beam lithography (EBL) is used to change the properties of the photoresist and creates the desired patterning. EBL requires additional equipment including the scanning electron microscope (SEM).

Figure 3: Fifteen process steps for fabrication of a PSL biosensor

Figure 4 shows film layers and its layers' order. The base layer is the silicon wafer with deposited layers of Cr, Au and PMMA.

Figure 4: Layers of film

After all etching is completed, PSL nanoparticles are assembled using electrophoresis to drive the particles into desired positions. PSL nanoparticles are supplied by Duke Scientific, Inc. The PSL nanoparticles have a stable ξ-potential over a wide range of pH in the aqueous solution. The size range for PSL nanoparticles is 50-200.

For the fabrication of these biosensors, the template is first patterned with arrays of two different size vias that provide size-selective assembly of two different particle sizes (Figure 5a) and described in Figure 4. Then a sequential assembly process sorts different size NPs into different locations. In first step, the patterned template is submerged into the suspension including larger sized NPs. These NPs can only fill the larger vias, because they do not fit in the smaller vias. The same template with the assembled larger nanoparticles is then submerged into another suspension with smaller size NPs that fill the smaller vias (Figure 5b). The same sequential assembly method can be used to sort differently sized nanoparticles by patterning the template with more variously sized vias. It is possible to functionalize different sized NPs with different antibodies, and through a sequential assembly process, the multiple detection capacity of the biosensors is increased. PSL nanoparticles in biosensors have a very high surface to volume ratio compared to the plates in enzyme-linked immunosorbent assay (ELISA) sensors that are currently the commercially available sensors. There are more antibodies per surface area for PSL nanoparticle based biosensors, which results in higher and stronger signals and improves the sensitivity of the biosensor. Also unlike sensing devices using well-plates which need high blood volume for testing, the nanoparticle biosensor chips scale to micron dimensions, requiring less blood volume for testing aspects. The fabrication method to pattern the template determines where the nanoparticles are placed and provides more control as to where the signals come from, which results in improvement of the biosensor sensitivity (Siavoshi, Yilmaz et al. 2011).

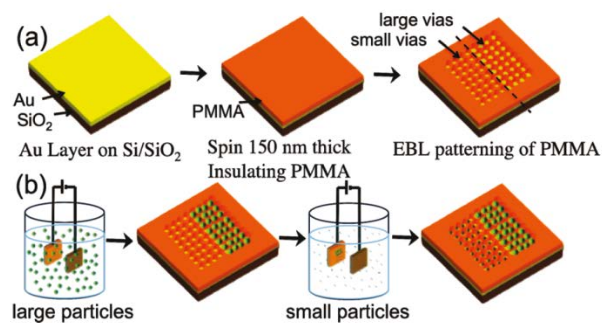


Figure 5: Schematic diagram of (a) template fabrication and (b) sequential electrophoretic assembly process (Siavoshi, Yilmaz et al. 2011).

3 LIFE CYCLE ASSESSMENT METHODOLOGY

Life Cycle Assessment **(**LCA) is a tool for assessing, investigating, and determining the potential environmental impacts from any manufacturing process, product, and service. It consists of four stages: goal definition and scope, inventory analysis, impact assessment and interpretation. Using LCA techniques, an inventory of relevant energy and material inputs and environmental releases is compiled and evaluated to identify the impact associated with each corresponding input. Life cycle assessment methodology is shown in Figure 6.

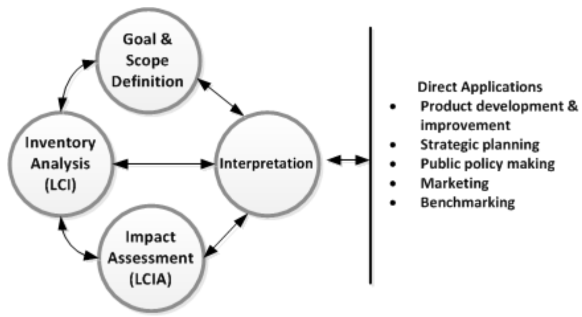


Figure 6: Life cycle assessment methodology (Organization 2006)

3.1 Goal Definition and Scope

The first phase, goal definition and scope, defines the purpose and evaluates the manufacturing of the particular application which is a biosensor in this study. The scope of this study is to evaluate only the manufacturing stage of PSL biosensors -- a cradle-to-gate approach.

3.2 Life Cycle Inventory

Life Cycle Inventory (LCI) is a data collection phase of LCA during which energy, raw materials, emissions, wastes, and releases for the entire process (Marry Ann Curran 2006). To evaluate the environmental impacts of fabrication of PSL biosensor, LCI data were collected by observing each manufacturing step. All reported parameters such as input data, energy consumption, emissions, and wastes are based on lab scale in this paper. The energy use was calculated based on power supply and time of use of equipment. All the operation information related to equipment was collected from user manuals or contacting the companies that supplied the equipment. The operation time of equipment was documented, and idle time was excluded from the calculations. All LCI data were entered into SimaPro^{TM} software to analyze and assess the environmental impacts.

The following input assumptions were made within SimaPro™:

- Electricity input as "Electricity, medium voltage, at grid/US"
- The electricity mix for U.S energy was assumed to be 30% coal, 24% natural gas, 21% crude oil, 16% hydropower, and 9% nuclear (Lindsay J. Dahlben 2009).
- Output Ar and CHF_3 air emissions were not included.
- Hazardous waste was input as "disposal, hazardous waste, 25% water, to hazardous waste incineration".
- Mixed wastewater to treatment for lab-scale fabrication input as "Treatment, sewage, to wastewater treatment, class 5," where a class 5 capacity denotes a small size municipal wastewater treatment plant (Lindsay J. Dahlben 2010).

Tables 1 and 2 show the energy and categorized input and output materials for each 3" silicon wafer used in the fabrication of a PSL biosensor.

Table 1: Total mass of input materials

ENERGY	
	[kWh/wfr]
	42.76
INPUT MATERIAL	
	[kg/wfr]
Acids/etchants & bases	0.3411
Gases (N2, O2, Ar)	0.365
Photoresist (PMMA + SU-8)	0.0025
Metals (Au, Cr)	0.00145
Solvents (acetone...)	0.291
Water (deionized)	8.2591
PSL nanoparticles	1.68E-18
INPUT TOTAL	**9.2601**

Table 2: Total mass of output materials

OUTPUT MATERIAL	
	[kg/wfr]
Mixed waste water to treatment	8.6001
Air emissions	0.365
Hazardous Waste	0.2675
PSL nanoparticles	1.68E-18
OUTPUT TOTAL	**9.2326**

3.3 Life Cycle Impact Assessment

The evaluation of potential human health and environmental impacts of the resources and emissions that were identified in the inventory phase, are undertaken in the third phase, life cycle impact assessment (LCIA). SimaPro^{TM} has a comprehensive database and libraries used to calculate the contributions to recognized impact categories, including: carcinogens, respiratory organics, respiratory inorganics climate change, radiation, ozone layer depletion, ecotoxicity, acidification /eutrophication, land use, mineral depletion, and fossil fuels.

The impact assessment selected to analyze the PSL biosensor fabrication processes was Eco-indicator 1999 H (EI99) method. In this method, all inventory data are classified by three themes: the damage to human health, ecosystem quality, and fossil resources.

4 RESULTS

The characterization and normalization results of the impact assessment of the lab scale fabrication for the PSL biosensor are shown in Figure 7 and Figure 8. These results were obtained by using SimaPro^{TM}.

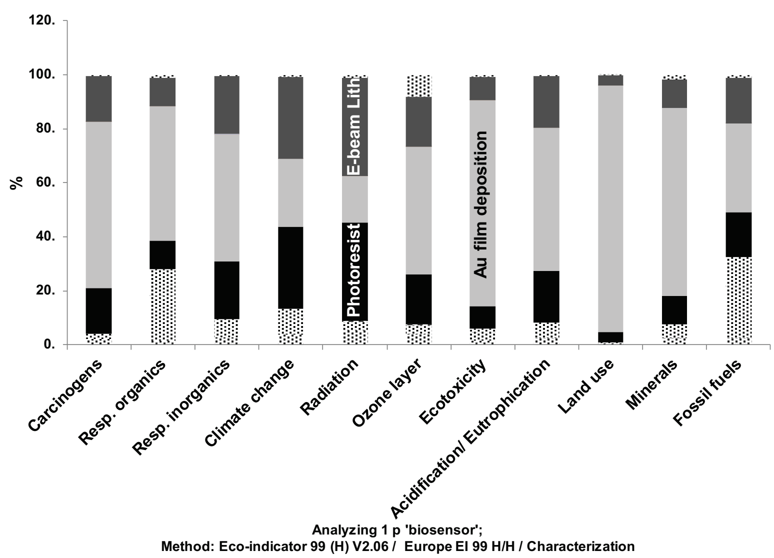


Figure 7: Biosensor characterization results show contributions primarily from three process steps: photoresist (black), E-beam lithography (dark gray), and Au film deposition (light gray), with all other process steps indicated by checkered gray.

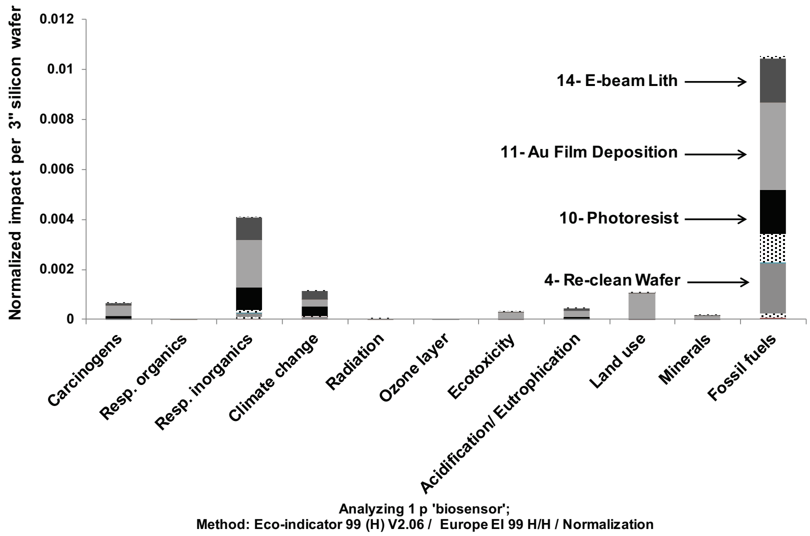


Figure 8: Biosensor normalized results indicating fossil fuels as the greatest contributor based on specific steps shown in Figure 4.

Figure 7 illustrates the fabrication steps that show the greatest contribution to each impact category for lab-scale PSL biosensor fabrication. The impacts from each step are sequentially ordered from the bottom of each impact category to the top. All impact categories that are affected by the wafer fabrication process have a total impact characterization of 100 % (Lindsay J. Dahlben 2010).

Step 11, Au film deposition using e-beam evaporation, shows the greatest contributions to all impact categories. Overall, process steps 10, 11, 14 (photoresist, electron beam lithography, and Au film deposition, respectively) are the three main processes which use the most energy during the manufacturing process and drive the environmental burden of PSL biosensor fabrication (Lindsay J. Dahlben 2010).

To determine and identify the relative contribution from the input materials to each environmental impact category, the result is normalized, as shown in Figure 8. The x-axis indicates the impact categories and the y-axis represents the normalized value corresponding to those categories. Results indicate that fabrication of PSL biosensors shows impacts related to fossil fuels, respiratory airborne inorganics, and climate change. Again, step 11, Au film deposition, dominates all of these impacts. The impact from airborne inorganics is due primarily to blasting and burning diesel in the Au refining processes and due to the use of sulfuric acid in pre-diffusion cleaning and piranha etches. The impact from fossil fuels is dominated by processes that require energy-intensive equipment such as a wet bench for cleaning. Fossil fuel impacts are due to the natural gas and crude oil production required for Au processing. There are also impacts on climate change due to CO_2 releases from the use of energy.

5 SUMMARY AND FUTURE WORK

As the field of nanotechnology matures, the focus shifts to implementation and commercialization. To successfully implement nanotechnology and nanoproducts into society, the environmental effects of nano-enabled products and materials must be understood, with a significant challenge to determine the effects of nanomaterials and nanomanufacturing on the environment and human health.

Results from a Life Cycle Inventory (LCI) of a biosensor fabricated with PSL nanoparticles are reported. Results indicate that fabrication of PSL biosensors shows impacts related to fossil fuels, respiratory airborne inorganics, and climate change. The specific toxicological impacts of nanoscale PSL particles are not available, hence are not included in results. Use of SimaPro™ software enables first order prediction of the environmental footprint of the processes, utilizing software databases to calculate the contributions to a set of recognized impact categories from the inventory data only for fabrication phase of the product. Results provide 1) a first order environmental footprint on the manufacturing process before scale-up, and 2) insights on potential process improvements given the uncertainty in regulatory constraints for nanomaterials.

Regulations will have the power to limit production, affect methods of manufacturing, or stop production altogether based on risk assessment. The risk assessment process for nanomaterials, as with for chemicals, is to identify the hazards of a substance, determine the levels of exposure, evaluate the severity of the hazardous effects, and make a quantitative estimation of probability. Such assessment of risk for nanoparticles is difficult, because so little conclusive evidence is available on adverse effects. This study investigated only the fabrication phase of a nanoparticle biosensor, and again, no specific toxicological impacts of nanoscale PSL particles are yet available. In future work and before scale-up of manufacturing, the life cycle investigation will be extended beyond the manufacturing phase to consider use and end-of-life.

To define the potential profitability and commercial viability of manufacturing scale-up of PSL biosensors, process-based cost models will be developed using life cycle inventories from the lab scale processes. With more detailed information on both the manufacturing cost and potential environmental impacts, more informed decisions regarding nanofabrication can be made, upon which interpretation, sensitivity analysis, and improvement to the processes can be assessed.

Zheng, B., Xie, S., Qian, L., Yuan, H., Xiao, D. and Choi, M. M. F. (2011): Gold nanoparticles-coated eggshell membrane with immobilized glucose oxidase for fabrication of glucose biosensor, in: Sensors and Actuators B: Chemical, Vol. 152, pp. 49-55.

[2] Li, Y., Wei, Y., Shi, G., Xian, Y. and Jin, L. (2011): Facile Synthesis of Leaf-Like CuO Nanoparticles and Their Application on Glucose Biosensor, in: Electroanalysis, Vol. 23, pp. 497-502.

[3] Vaddiraju, S., Tomazos, I., Burgess, D. J., Jain, F. C. and Papadimitrakopoulos, F. (2010): Emerging synergy between nanotechnology and implantable biosensors: A review, in: Biosensors and Bioelectronics, Vol. 25, pp. 1553-1565.

[4] Carrascosa, L. G., Moreno, M., Álvarez, M. and Lechuga, L. M. (2006): Nanomechanical biosensors: a new sensing tool, in: TrAC Trends in Analytical Chemistry, Vol. 25, pp. 196-206.

[5] Wen-Tso, L. (2006): Nanoparticles and their biological and environmental applications, in: Journal of Bioscience and Bioengineering, Vol. 102, pp. 1-7.

[6] Jianrong, C., Yuqing, M., Nongyue, H., Xiaohua, W. and Sijiao, L. (2004): Nanotechnology and biosensors, in: Biotechnology Advances, Vol. 22, pp. 505-518.

[7] Kim, T. H., Park, I. K., Nah, J. W., Choi, Y. J. and Cho, C. S. (2004): Galactosylated chitosan/DNA nanoparticles prepared using water-soluble chitosan as a gene carrier, in: Biomaterials, Vol. 25, pp. 3783-3792.

[8] Ibtisam E, T. (2009): Biosensors for cancer markers diagnosis, in: Seminars in Cell & Developmental Biology, Vol. 20, pp. 55-62.

[9] Siavoshi, S., Yilmaz, C., Somu, S., Musacchio, T., Upponi, J. R., Torchilin, V. P. and Busnaina, A. (2011): Size-Selective Template-Assisted Electrophoretic Assembly of Nanoparticles for Biosensing Applications, in: Langmuir, Vol. 27, pp. 7301-7306.

] Olapiriyakul, S. (2010): End-of-Life Analysis of Nanotechnology Products, in: Mechanical and Industrial Engineering, Doctoral of Philosophy in Industrial Engineering, pp. 170

[11] Ray, P, C., Yu, H., Fu, F. (2009): Toxicity and Environmental Risks of Nanomaterials: Challenges and Future Needs, in: Environmental Science and Health Part, Vol. 27, pp. 36.

[12] Gottschalk, F., Nowak, B., Gawlik, B (2010): Report on Exposure Scenarios and Release of Nanomaterials to the Environment, in: nanex-project.eu/index.php/public-documents/.../90-nanexwp5final

[13] Hankin, S. (2010): Lithium-Ion Batteries and Carbon Nanotubes, in: www.safenano.org

[14] Environmental Protection Agency. (2011): Summery of the ToxicSubstancesControlAct http://www.epa.gov/lawsregs/laws/tsca.html

[15] Stander, L. and Theodore, L. (2011): Environmental Implications of Nanotechnology—An Update, in: International Journal of Environmental Research and Public Health, Vol. 8, pp. 470-479.

[16] Musee, N. (2011): Nanowastes and the environment: Potential new waste management paradigm, in: Environment International, Vol. 37, pp. 112-128.

[17] Curran, M, A. (2006): Life Cycle Assessment: Principles and practice, in: http://www.epa.gov/nrmrl/lcaccess/lca101.html

[18] Dahlben, L, J. and Isaacs, J, A. (2009): Environmental Assessment of Manufacturing with Carbon Nanotubes, in: The International Symposium on Sustainable Systems and Technology, pp. 5

[19] Dahlben, L, J. and Isaacs, J, A. (2010): Investigation of the Environmental Implications of the CNT Switch through its Life Cycle, in: Industrial Engineering, Master of Science, pp. 116