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Advancing Life-Cycle Assessment Techniques

Marlo Raynolds

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A thesis submitted to the Faculty of Graduate Studies and Research in partial fulfillment of the requirements for the degree of Doctor of Philosophy

Department of Mechanical Engineering

Edmonton, Alberta

Fall 1999



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Box 7558 Drayton Valley, AB, T7A 1S7 "Whatever you may do may seem insignificant, but it is most important that you do it."

- Gandhi

University of Alberta

Faculty of Graduate Studies and Research

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled "Advancing Life-Cycle Assessment Techniques" submitted by Marlo Raynolds in partial fulfillment of the requirements for the degree of Doctor of Philosophy

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Dedicated to my parents for their love and everlasting support.

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Abstract

Life-cycle assessment (LCA) is a decision analysis tool for evaluating the relative environmental performance of competing services, products or system designs. LCA uses a systems approach by quantifying material and energy inputs and environmental outputs throughout the life-cycle of a given product or service from "cradle-to-grave". This quantification is called the life-cycle inventory (LCI) stage of LCA. To be of greatest value, the decision-maker will require an indication of the uncertainty and sensitivity associated with the LCI.

This work presents six tools developed to improve the rigor in LCI: 1. the Relative Mass-Energy-Economic (RMEE) method for system boundary selection and estimation of uncertainty due to system boundaries; 2. Marginal Sensitivity Analysis; 3. Monte Carlo Analysis for Calculating Error Propagation; 4. Monte Carlo Analysis for Combining Data Uncertainty and System Boundary Uncertainty; 5. Calculation of Confidence in Relative Performance; and 6. Uncertainty Reduction Analysis.

The RMEE method of system boundary selection ensures comparable system boundaries are selected for a fair comparison between systems. It also provides a practical method of estimating uncertainty due to system boundary selection. The RMEE method defines a system boundary by Z_{RMEE} which is the ratio of mass, energy, and economic value of any input in the system to the functional unit of the LCA. The underlying assumption for the RMEE method is a direct relationship between the magnitude of environmental outputs from a unit process and the mass, energy and economic value of its products. As a result, RMEE has been developed and tested specifically for evaluation of energy systems where combustion-related emissions are of primary interest.

Marginal Sensitivity Analysis and Uncertainty Reduction Analysis are tools, which identify where time and resources should be spent on collecting data to improve the LCI. Monte Carlo Analysis provides a rigorous means to evaluate the propagation of error in LCI. This tool provides a flexible and quantitative method, which can handle nonnormal, asymmetrical distributions of inventory data. Using the above techniques, a confidence level in relative performance of systems can be calculated.

The tools presented for making LCI more effective are integrated and demonstrated on a case study of four different automotive fuels: reformulated gasoline, compressed natural gas, and two different sources of 85% blended ethanol (E85).

Keywords:

life-cycle assessment (LCA), life-cycle inventory (LCI), cradle-to-grave, Monte Carlo Analysis, Relative Mass-Energy-Economic (RMEE), system boundary selection, automotive fuels, reformulated gasoline, natural gas, ethanol blended gasoline (E85)

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List of Abbreviations

ARP	Acid Rain Precursors	
CH ₄	Methane	
CNG	Compressed Natural Gas	
CO2	Carbon Dioxide	
DDGS	Distillers dried grains and solubles	
DQI	Data Quality Indicator	
E85	Ethanol blended gasoline (85% ethanol, 15% gasoline by volume)	
GHG	Greenhouse Gases	
GLO	Ground Level Ozone Precursors	
ISO	International Organization for Standardization	
LCA	Life-Cycle Assessment	
LCI	Life-Cycle Inventory	
MTBE	Methyl-Tertiary Butyl Ethyl	
N ₂ O	Nitrous Oxide	
NOx	Nitrogen oxides	
RFG	Reformulated Gasoline	
RMEE	Relative Mass-Energy-Economic	
SBS	System Boundary Selection	
UP	Unit Process	
VOC	Volatile organic compound	

List of Nomenclature

α	Significance level for T-test.
C _{ij}	Co-products of unit process i of type j.
Ei	Energy input to unit process i.
E _{i%}	Percentage of any given energy input (E_i) to the total energy inputs of a
	system (E _{SystemTotal}).
E _{Ratio}	The ratio of an energy input (E_i) to the total energy of the functional unit
	(E _{Total}).
E _{SystemTotal}	Total energy inputs to an LCA system.
ETotal	Total energy value of the functional unit.
Fr ⁱ	Frequency of the environmental output of system j in histogram bin i
H _a	Alternative hypothesis for T-test.
H _o	Null hypothesis for T-test.
M _i	Mass of input to unit process i.
M _{i%}	Percentage of any given mass input (M_i) to the total mass inputs of a system
	(M _{SystemTotal}).
M _{Ratio}	The ratio of a mass input (M_i) to the total mass of the functional unit
	(M _{Total}).
M _{SystemTotal}	Total mass of inputs to an LCA system.
M _{Total}	Total mass of the functional unit.
n	Number of unit processes in a system.
N	Number of bins in the histogram.
P _{Fn}	The product or service representing the functional unit.
Pi	Product or service from unit process i.
I _{ij}	Input to unit process i of type j.
M _{RMEE}	Mode of the distribution of Y _{ZMean.}
ri	95% confidence interval in the mean environmental output (x_i) of unit process i.
r _{data}	95% confidence interval for X _{zj}
r _{SysBndry}	95% confidence interval for Y _{zMean}

r _{Total}	Combination of the 95% confidence interval of r_{data} and $r_{SysBndry}$ and
	represents an approximation of the total uncertainty of an LCA.
S	Standard deviation for T-test.
S _{RMEE}	Standard deviation of the distribution of Y _{ZMean.}
Si	Market value of input to unit process i.
S _{Ratio}	The ratio of the market value of an input to a unit process (\mathbf{s}_i) to the total
	market value of the functional unit (\$Total).
STOL	Total market value of the functional unit.
Т	The T-statistic.
U	Mean value for T-test.
x _i	Environmental output of a given type from unit process i.
\mathbf{X}_{Zj}	Mean total environmental output of a given type (e.g. greenhouse gases)
	calculated for system j with system boundaries defined by Z_{RMEE} (Z).
X _{Zj} '	Approximation of the true mean environmental output after having adjusted
	X_{Z_j} with the RMEE factor Y_{ZMean} .
х	Total environmental output of a system which has not taken into account
	system boundary selection.
Y _{ZMean}	Mean fraction, expressed as a percent, of the actual total environmental
	outputs reported for a system with system boundaries defined by Z_{RMEE} (Z).
Y_{ZHigh}	The upper bound of the 95% confidence interval for Y_{ZMean} .
Y _{ZLow}	The lower bound of the 95% confidence interval for Y_{ZLow} .
Z _{RMEE}	The cut-off ratio used in the RMEE method of system boundary selection.

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Chapter 1

Introduction

Chapter 1 sets the context for this thesis, provides an introduction to life-cycle assessment, states the objectives of this research, and outlines the content of each chapter.

1.1 Setting the Context

As we enter the next century, engineering will increasingly be challenged to redesign our energy, material, service and economic systems to become cleaner, more efficient, and environmentally sustainable. The driving force for a "Sustainable Revolution" is a slow realization that we are pushing the limits of the Earth's tolerance of pollution, resource extraction, and population as indicated by climate change, depletion of water reserves, depletion of fish stocks, widespread deforestation, and a range of other "vital signs" [1]. A "Sustainable Revolution" requires holistic, long-term thinking where business and government take a "systems" approach to making decisions. Life-cycle assessment (LCA) is a decision making tool applicable to energy, material, service and economic systems which forces a systems analysis to make better informed decisions.

Over the past thirty years, life-cycle assessment methodologies have developed to become widely recognized as an effective decision making tool. This is indicated by their widespread use across numerous industries including automotive, utility, forestry, telecommunications, and materials [13][14] [19]. As a result, the International Organization for Standardization (ISO) is developing international guidelines for LCA within its ISO 14000 Environmental Management Standards [8]. The ISO process has provided international language and a standard framework for how LCA may be completed. ISO 14040 defines LCA as "a technique for assessing the environmental and potential impacts throughout a product's life" [8].

Originally the objective of this research was to evaluate a broad range of existing and developing automotive fuels and technologies using life-cycle assessment (LCA). It became apparent that the current methodologies of LCA were not rigorous enough to confidently evaluate the life-cycle performance of competing fuels or any energy system for that matter. A major gap in LCA techniques was found in evaluating the uncertainty of results in the life-cycle inventory (LCI) stage of LCA. It was soon found that the current techniques for selecting system boundaries in LCA did not provide a repeatable and practical method, nor provide a means for estimating uncertainty due to system

boundary selection. In addition, it is the opinion of the author that practical tools did not exist to properly evaluate the propagation of error in the data collection stage, called the life-cycle inventory (LCI) stage, of LCA.

As a result, the focus of this research shifted from an engineering analysis of the environmental performance of automotive fuels, to engineering tools to better complete LCA. The primary objective of this research is to develop rigorous tools for system boundary selection, identifying sensitive data values, and evaluating uncertainty in LCI. This research has resulted in the development and testing of six tools to advance LCA:

- 1. The Relative Mass-Energy-Economic (RMEE) Method for System Boundary Selection,
- 2. Marginal Sensitivity Analysis,
- 3. Monte Carlo Analysis for Calculating Error Propagation in LCA Data,
- 4. Monte Carlo Analysis for Combining Data Uncertainty and System Boundary Uncertainty,
- 5. Calculation of Confidence in Relative Performance, and
- 6. Uncertainty Reduction Analysis.

These six tools were developed and tested first on random, fully defined systems. Next, these individual tools were integrated with the intention of contributing a practical and rigorous method for completing the inventory assessment stage of LCA. With this newly developed method, this research circled back to its original objective of evaluating automotive fuels. In the end, an analysis of the relative life-cycle environmental performance of three automotive fuels has been accomplished. More importantly, the techniques of LCA have been advanced to better select system boundaries, identify sensitive data values, and evaluate uncertainty in results. The RMEE method of system boundary selection has been designed and tested specifically for LCA studies investigating common combustion related air emissions from energy and product systems. The remainder of the tools are suitable for broader application in LCA.

The remainder of Chapter 1 describes LCA methodologies, describes how LCA fits into decision analysis, provides a brief history of LCA, identifies the current challenges to overcome in the field of LCA, and defines the objectives of this research.

1.2 Decision Analysis and Life-Cycle Assessment

Decision analysis encompasses any tool or technique designed to systematically assess a situation and provide the decision-maker with more complete information. Decision analysis techniques do not provide answers to decisions, but they provide information to decision-makers. As quoted by Bunn (1984) (found in [2]):

"the basic presumption of decision analysis is not at all to replace the decision maker's intuition, to relieve him or her of the obligations in facing the problem, or to be, worst of all, a competitor to the decision maker's personal style of analysis, but to complement, augment, and generally work alongside the decision maker in exemplifying the nature of the problem. Ultimately, it is of most value if the decision maker has actually learned something about the problem and his or her own decision-making attitude through the exercise."

The objective of decision analysis is to lead to better decisions. The current global economic, social, and environmental systems result in the need to make very complex inter-related decisions. These decisions can affect many people, involve various trade-offs, and must be made with inherent uncertainty. Decision analysis tools provide a systematic approach to organizing complex problems and provide insight on the situation, uncertainty, objectives, and trade-offs between competing alternatives [2].

The general framework for any decision analysis tool involves five steps [2][17]:

- 1) identify the decision to be made,
- 2) identify alternatives,
- 3) decompose the model and problem,
- 4) evaluate the results, and
- 5) make the decision.

Life-cycle assessment is a decision analysis tool, which includes each of these five steps. Figure 1.1 shows the specific steps in LCA and where they fit into the generic framework of decision analysis. A description of each step within LCA is provided below.

KT Analysis and LCA

KT analysis is a business decision-making tool developed by Kepner-Tregoe, Inc. which provides a "systematic process for making a choice" and is quite widely applied in industry [11].

The KT decision analysis process has four basic stages [11]:

- 1. Clarify Purpose
 - State Decision
 - Develop Objectives
 - Classify Objectives into Musts and Wants
 - Weight the Wants
- 2. Evaluate Alternatives
 - Generate Alternatives
 - Screen Alternatives through the Musts
 - Compare Alternatives against the Wants
- 3. Assess Risks
 - Develop Adverse Consequences
 - Assess Threat
- 4. Make Decision
 - Make best balanced choice.

Like the KT approach, LCA can be applied to a broad range of decisions. Both can be applied at differing levels of intensity with very similar general steps in completing either analysis as shown in Table 1.1.

Table I.I. Company	VII VII ILL AMBIYSIS BUU LCA
KT Analysis Step	LCA Step
Clarify Purpose - state decision	Goal and Scope Definition
Evaluate Alternatives	Inventory Assessment
Assess Risks	Impact Analysis/ Design Improvement
Make Decision	Make Decision

Table 1.1: Comparison of KT Analysis and LCA

How is LCA Different?

The fundamental difference between LCA and other decision analysis tools, such as KT Analysis is that LCA takes a systems approach to collecting and analyzing information for decision making. This systems approach involves comparing options based on the entire life-cycle, from "cradle-to-grave". LCA is specifically intended to compare the performance of competing systems which provide a specific service or product [8]. Over the past thirty years, it has been increasingly recognized that "in a society which is producing more people, more materials, more things, and more information than ever before, systems engineering is indispensable in meeting the challenge of complexity." [15].

Furthermore, LCA is particularly well suited for comparing systems based on their relative environmental performance. The primary objective of LCA is to present the decision-maker with a complete system analysis of the environmental performance of competing products or services. The results of an LCA provide the decision-maker with more complete information on key environmental parameters, relative performance, and pointers to areas within the system to focus on improvement.

In short, LCA is a decision analysis tool, which uses a systems analysis approach and is primarily focused on relative environmental performance. Life-Cycle Assessment is defined by ISO 14040 as:

"a technique for assessing the environmental and potential impacts throughout a product's life".

Various consultants have adapted the concepts of life-cycle thinking to form business decision making tools which combine environmental and economic aspects. An example, is the Pembina Institute's method called Life-Cycle Value Assessment [www.pembina.org]:

"Life-Cycle Value Assessment (LCVA) is a business analysis and decisionmaking tool that combines potential environmental impacts for the full life-cycle of a product or system, with financial cost-benefit information, for better decisions."



Figure 1.1: Comparison of General Frameworks for Decision Analysis and LCA [2][8]

LCA Methodology

The general framework for LCA as presented by the ISO 14040 "Environmental management – Life cycle assessment – Principles and framework" [8] is shown in Figure 1.2. Although many variations of LCA exist, they all generally follow the general framework.

For the work presented here, a slight modification to Figure 1.2 was made with respect to the flow of the four major steps in LCA. The modifications, shown in Figure 1.3, assume the LCA practitioner proceeds to Impact Assessment and Interpretation only after an Inventory Analysis is complete. Furthermore, it is assumed Inventory Analysis is revisited only after Goal and Scope Definition is revisited. This flow is illustrated in Figure 1.3 by the arrows returning to Goal and Scope Definition. The reasoning behind this is the purpose of Goal and Scope Definition is to define what is to be quantified. If the results of the Inventory Analysis do not allow for an impact analysis and interpretation (decision making), then the goal and scope must be revisited prior to changing the inventory. The primary objective of this research is to develop rigorous tools for Inventory Analysis to select system boundaries, to identify sensitive data points in the inventory, and to provide the decision-maker with an indication of the confidence in the results from the inventory.

Goal and Scope Definition

Goal definition and scoping are concerned with clearly describing the objectives and extent of the LCA to be completed. The goal clearly states the intended application, the audience, and the reason for completing the LCA.

As described by ISO 14040, scoping requires the following to be considered and clearly described [8]:

- the functions of the product system, or, in the case of comparative studies, the systems;
- the functional unit;
- the product system to be studied;

- the product system boundaries;
- allocation procedures;
- types of impact and methodology of impact assessment, and subsequent interpretation to be used;
- data requirements;
- assumptions;
- limitations;
- initial data quality requirements;
- type of critical review, if any;
- type and format of the report required for the study.

The scoping stage of LCA initiates the process of thinking through the entire life-cycle of a product or service system from raw material acquisition, through production, use and maintenance, to final disposal.

Inventory Assessment

Inventory assessment involves collecting and calculating data to quantify relevant inputs and outputs throughout the life-cycle system. These inputs and outputs include materials, energy, and releases to the environment through air, water, or land. Completion of the Inventory Assessment stage of LCA results in a "life-cycle inventory" (LCI). This provides information for the impact assessment and interpretation, which ultimately lead to the decision [8]. The six tools developed through this research fit into the stage of Inventory Assessment and are designed to address system boundary selection and uncertainty analysis in the inventory.

Impact Assessment

The objective of the impact assessment phase is to evaluate the significance of potential environmental impact based on the inventory assessment. This normally includes a process of assigning and modeling inventory data to environmental impact stressor categories. The methodological and scientific framework for how impact assessment should be completed is still in development [8]. Advancing the tools of impact assessment is beyond the scope of this research.



Figure 1.2: ISO 14040 Life-cycle Assessment Framework [8]



Figure 1.3: Modified Flow of LCA Steps
Interpretation

The interpretation phase of LCA involves bringing the results of the inventory assessment and the impact assessment together to reach conclusions and recommendations based on the goal of the LCA. These conclusions are fed into the decision making process. Methods for LCA interpretation are still evolving through the ISO process. Advancement of these methods is beyond the scope of this research.

Although the International Organization for Standardization has been involved, since 1993, in developing the framework for LCA, a number of challenges still remain in defining specific components within the methodology to ensure credible LCAs are completed. These challenges include:

- 1. system boundary selection,
- 2. sensitivity analysis,
- 3. uncertainty anlaysis,
- 4. data quality indicators,
- 5. evaluation of different environmental impacts, and
- 6. interpretation of results for consistent decision making.

Because the ISO 14000 series of guidelines on environmental management are receiving international attention by government and industry, life-cycle assessment is becoming more widely known as an environmental management tool. It therefore becomes important to address the above challenges as LCA becomes more broadly applied in decision making.

1.3 Milestones of Life-cycle Assessment

The first comprehensive, environmental life-cycle assessment type of analysis is considered to have been conceived in 1969 by Harry E. Teasley [3][6]. At the time, Teasely was managing the packaging operations for The Coca-Cola Company and was deciding which type of beverage packaging to use[6]. He wanted to quantify the energy, material and environmental consequences of the entire life-cycle of the packaging from raw materials to final disposal [6]. To complete this work, Teasely approached the Midwest Research Institute (MRI), a contract research organization, who completed an evaluation of a number of packaging options available to The Coca-Cola Company. This first study was not called an LCA but a "Resource and Environmental Profile Analysis" (REPA) [3][6]. Although the results were never published, the study showed advantages to switching from glass to plastic bottles [6]. Two of the primary researchers at MRI, Bob Hunt and Bill Franklin, went on to complete other REPA studies for other companies and government [3][6].

During the early 1970's a number of REPA studies were completed on a broad range of consumer products including meat trays, napkins, towels, milk containers, beer containers, and diapers [3][6]. At this time, the focus of evaluation was on waste management issues [6]. Due to the energy crisis, by 1975 the focus shifted from waste management to energy consumption [6]. A number of major REPA studies were sponsored by the U.S. government and industry [3][6].

During the 1980's the public sector lost interest in REPA while private companies continued to apply life-cycle thinking to product design [6]. As a result, there are very few published studies during the 1980's [3]. Starting in the late 1980's, a re-awakening of interest in life-cycle thinking began with greater public interest in environmental issues [6].

In 1991, the term "Life-cycle Assessment" (LCA) was born when the Society of Environmental Toxicology and Chemistry (SETAC) published "A Technical Framework for Life-Cycle Assessment" [4][6]. SETAC was instrumental in defining the terminology and initial methodologies for LCA [6]. An explosion of activity in the field of LCA has occurred during the 1990's both in industry and government [6]. For a more complete history of LCA refer to CURRAN's textbook [3] and the paper presented by HUNT and FRANKLIN [6].

The LCA framework developed through SETAC provided qualitative methods for selecting system boundaries and evaluating data quality [4][5]. Through the 1990's LCA has evolved to include quantitative methods for system boundary selection and data quality [3][10][7][3]. It is the author's opinion that none of the existing methods for system boundary selection are rigorous and practical in use. This is demonstrated in Chapter 2 where a literature review and assessment of existing methods is completed. In addition, there appears to be no published work or current research on the relationship between system boundary selection and uncertainty in the results of LCA. In general, this source of uncertainty tends to be completely ignored by current LCA work. An objective of this research is to develop a practical means of incorporating uncertainty due to system boundary selection into the results of LCA.

Starting in 1993, the International Organization for Standardization (ISO) brought together LCA experts from all over the world to develop international guidelines on how to complete LCA. The recently published ISO 14040 and 14041 documents entitled "Environmental management – Life-cycle assessment – Principles and Framework" and "Environmental management – Life cycle assessment – Goal and scope definition and inventory analysis" are the guidelines covering both system boundary selection and uncertainty analysis [8][9]. With respect to system boundary selection, the ISO guidelines recognize the importance of ensuring comparable system boundaries are selected in a quantitative manner [8]. However, as the author argues in Chapter 2, the method suggested by ISO is not practical. To provide a more rigorous and practical approach to system boundary selection for LCA, the author has invented the Relative Mass-Energy-Economic Method for system boundary selection.

The importance of properly assessing uncertainty in the results of an LCA is clearly expressed in the ISO guidelines [8][9]. ISO recommends ranges or probability distributions be used to determine the uncertainty in results but provides no guidelines on how to complete uncertainty analysis [9]. Here, the author has developed a means to apply Monte Carlo Analysis with the intent to provide a practical and rigorous approach to evaluating the propagation of error in life-cycle assessment. KENNEDY et al [10] completed initial research on the application of Monte Carlo Analysis to LCA and in doing so identified two areas requiring further research:

- "The final impact of the cascading uncertainty associated with the aggregation of input data from multiple levels of LCA inventory modeling requires additional analysis.", and
- 2. "a method needs to be developed to anlayze the LCA inventory model input data to identify those data elements that significantly contribute to the variance of the results." [10]

The objective of the research presented here is to develop a practical method to use Monte Carlo Analysis for uncertainty analysis and develop a method to analyze inventory data in order to identify the most significant data points.

Because LCA is being more broadly used, the need for a rigorous method of system boundary selection and uncertainty analysis will be in greater demand. To meet this need, the author has built upon the work of others over the past to develop an integrated approach to selecting system boundaries and estimating total uncertainty in LCA.

1.4 Challenges in Life-Cycle Assessment and the Objectives of this Research

Professional experience in the field of LCA is evolving. In any professional practice, such as engineering or medicine, expertise is relied upon to combine professional judgement and sets of rules for decision making. As expertise develops, the profession evolves to develop and apply tools to supplement experience alone. A professional field is generally considered to require a common educational background, a minimum amount of experience, and a similar code of ethics. In established professions, this is often regulated by law or certification by a professional body. The field of LCA is currently best defined by the International Organization for Standardization (ISO), which does not require any certification or qualifications for practitioners of LCA. Through ISO 14000, LCA practitioners are moving experience towards a set of guidelines for completing LCA. As the field of LCA continues to evolve, additional tools will be developed and accepted by the profession to supplement professional judgement. Nevertheless, like any systems analysis or decision analysis tool, LCA continues to involve a combination of 'art' and 'science' [16]. Like business decision making, LCA will always involve judgement from the practitioner. The field must evolve specific tools to manage uncertainty and operate on an agreed set of rules in order to arrive at repeatable results. The author's objective of this research is to advance the techniques of LCA to lead to more repeatable LCA studies. In addition to the techniques developed here, LCA practice must strive to ensure transparency in method and data, as well as enhanced external verification.

First, how do we define 'system'? The traditional definition of a system is [18]:

"a collection of parts and relations between the parts such that the behavior of the whole is a function not only of the behaviors of the parts, but also of the relations among them". In other words, a system involves interconnections of elements where, if a change is made to any one element, there are likely to be many subtle consequences. The behavior of a system is determined by the rules describing the relation between inputs and outputs [18].

Next, what is 'system simulation'? In general usage, simulation is defined as an act or process that provides the appearance of some part of reality [12]. As Maisel (1969) stated, the purpose of simulation is "to attain the essence without the reality" [12]. Maisel (1972) provides a more operational definition of system simulation:

"simulation is a numerical technique for conducting experiments on a digital computer, which involves certain types of mathematical and logical models that describe the behavior of a business or economic system (or some component thereof) over extended periods of time."[12]

For the purpose of life-cycle assessment, system simulation is interested in describing the behavior of a product or service system. LCA quantifies 'behavior' of the system based on its environmental performance.

Shannon (1975) describes simulation as one of the most powerful analysis tools available for design and study of complex processes or systems, and defines simulation as

"the process of designing a model of a real system and conducting experiments with this model for the purpose either of understanding the behavior of the system or of evaluating various strategies for the operation of the system."[16].

It is in the development of the model where 'art' and 'science' meet, providing significant challenges for the analyst who must balance simplicity against reality.

The major advantage of system simulation is the ability to study a real or proposed system without actual development or modification of the system. The major obstacle to

system simulation, and therefore LCA, is ensuring the simulation represents reality in enough detail to provide meaningful information to the decision-maker. Simulation is capable of giving very valuable information to decision-makers, but it is also capable of providing very wrong and deceiving results [16].

LCA has a number of challenges to overcome in order to ensure its method of system simulation provides valuable information for decision making. The author believes the current major methodological challenges for LCA to overcome are:

- 1. system boundary selection,
- 2. uncertainty analysis, and
- 3. impact analysis.

All three challenges currently involve a large degree of subjectivity or "art" [8]. Current professional practices for these components of LCA are not consistent or well defined. As a result, ISO 14000 has not been successful in developing guidelines to address these challenges. With the development of trading systems for greenhouse gases both nationally and internationally, LCA techniques may become a very important tool to quantify true emission reductions. To accomplish this, an accepted method of system boundary selection and uncertainty analysis is required. This research is primarily focused on addressing two of the three major challenges of LCA: system boundary selection and uncertainty analysis.

Objectives of this Research

The objective of this research is to improve the engineering tool of LCA to provide better decision making information on the relative environmental performance of options. The research does not develop an entirely new LCA methodology, but advances the stage of Inventory Assessment to better select system boundaries, to identify sensitive data values, and to evaluate uncertainty in results. Because LCA is an engineering tool, the methods developed here have continuously kept in mind the need to ensure the techniques are practical.

It is the objective of this thesis to contribute to the field of LCA as follows:

- 1. Develop a quantitative, repeatable, and practical method of selecting system boundaries for comparison of life-cycle systems;
- 2. Develop an effective and rigorous method for identifying the most sensitive data values in an LCA;
- 3. Develop a quantitative framework for assessing the propagation of data uncertainty in LCA system simulation and combine this uncertainty with uncertainty due to system boundary selection to provide an estimate of the total uncertainty in inventory results;
- 4. Demonstrate these new methods of system boundary selection and uncertainty analysis on an energy system decision: automotive fuels.

The tools developed here are applicable to the inventory assessment stage of LCA studies. These tools have been developed with primary interest on air emissions from combustion processes throughout the life-cycle of energy systems. Decisions regarding energy systems may be made at various levels including new facility decisions, decision making for expansions or technology change outs in existing facilities, or policy decision making at the national or regional scale. The LCA practitioner must take caution in applying the RMEE system boundary selection tool, presented here, to systems where the environmental outputs are not directly proportional to the mass, energy or economic value of unit process products.

This research does not attempt to:

- advance the techniques of impact assessment and therefore does not attach values to potential impacts;
- develop techniques to estimate individual data point uncertainty. The methods here assume either statistical analysis or professional judgement have been used to provide an estimate in uncertainty of any particular data point;
- evaluate existing methods of allocating environmental outputs to multiple products from an individual unit process in a system. As shown in the case study in Chapter 6, allocation is completed using the economic value of products. In

other words, environmental emissions of a unit process are allocated to its various products based on the proportion of economic value each product generates.

In developing the tools presented here, a software package was developed using Microsoft Access and Visual Basic. This thesis presents the techniques developed and the methods used, but does not provide a detailed description of each module and algorithm in the software.

1.5 Description of Chapters

This thesis is organized into seven chapters, followed by two supporting appendices. Chapters 2 through 4 contain individual papers, which have been refereed and accepted for journal publication. Together they present the six tools developed by the author. Chapter 5 summarizes these six LCA tools and presents an integrated approach for their application in LCA. Chapter 6 is a paper presenting the application of the advanced LCA tools on three different fuels to evaluate their relative environmental performance based on emissions of greenhouse gases, acid rain precursors, and ground level ozone precursors. Chapter 7 presents conclusions drawn from this research. Appendix I is an additional refereed published paper presenting a case study on ethanol fuels. Appendix II provides a brief description of the computer software developed to test the tools on real and random systems. Table 1.2 presents a brief description of each chapter.

Chapter	
	Description
2.0 The Relative Mass-Energy-Economic (RMEE) Method for System Boundary Selection – Part 1: A Means to Systematically and Quantitatively Select LCA Boundaries	 A peer-reviewed published paper which: describes the challenges of system boundary selection for LCA, and current methods in use, and presents the RMEE system boundary methodology.
3.0 The Relative Mass-Energy-Economic (RMEE) Method for LCA System Boundary Selection – Part 2: Selecting the Boundary Cut-off Parameter and its Relationship to Overall Uncertainty	 A peer-reviewed published paper which: presents research on the relationship between the RMEE boundary cut-off parameter and uncertainty introduced to the results due to system boundary selection, describes the method of generating and modeling 800 different systems to identify a relationship, and presents a method for estimating the confidence one system results in less environmental emissions than another.
4.0 Assessing Uncertainty in Life-Cycle Assessment	
4.1 Application of Monte Carlo Analysis to Life-Cycle Assessment	 A peer-reviewed published paper which: introduces the various sources of uncertainty in LCA, describes existing methods for assessing uncertainty in LCA, and presents research completed on the appropriate use of Monte Carlo Analysis for calculating error propagation.
4.2 Additional Analysis of Monte Carlo Analysis Convergence	• Revisits and confirms convergence of the Monte Carlo Analysis modeling work presented in Chapter 4.2.
4.3 Non-Linearity in Modeling LCA	 Discussion of how the systems modeled in LCA become non-linear, leading to the need for a stochastic system of evaluation such as Monte Carlo analysis, discusses the marginal sensitivity method of sensitivity analysis, and compares the beta distribution to the normal distribution.

Table 1.2:Description of Chapters

Table 1.2. Description of Chapt	
Chapter	Description
5.0 Integrating the System Boundary and Uncertainty Analysis Tools into the Inventory Assessment Stage of LCA	• Presents the combination of the tools from Chapters 2,3, and 4 into a concise package for completing inventory assessment.
6.0 A Case Study Life-Cycle Assessment (LCA) Applying the Relative Mass- Energy-Economic (RMEE) Method of System Boundary Selection and Monte Carlo Analysis to Automotive Fuels	 A case-study chapter which: presents an application of the integrated tool set presented in Chapter 5 on various alternative automotive fuels including MTBE reformulated gasoline, ethanol blended gasoline (E85), and natural gas.
7.0 Conclusions	
	• Drawing from the various chapters, a set of conclusions from the research is presented.
Appendix I: Case Study – A Life-Cycle Assessment of Various Feedstocks for Ethanol Fuel	 A peer-reviewed published paper which: presents the research results of comparing corn, wheat and poplar trees as feedstock for producing ethanol fuel using life-cycle assessment.
Appendix II: Description of LCA Model	 Provides description of the model developed parallel to this research for modeling LCA systems, testing Monte Carlo Analysis, and completing RMEE.
Appendix III: Data Sources for Fuel Comparison	• Provides detailed input and output data used in modeling the fuel comparison of Chapter 6.

Table 1.2: Description of Chapters Continued

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Chapter 2

The Relative Mass-Energy-Economic (RMEE) Method for System Boundary Selection

Part 1: A Means to Systematically and Quantitatively Select LCA System Boundaries

Consistently selecting comparable system boundaries is essential for any fair comparison between competing systems. To ensure a rigorous method for system boundary selection in LCA, a repeatable and quantitative tool is required. Chapter 2 identifies the characteristics of a "good" system boundary selection method, reviews current practices in the field of LCA, and introduces the Relative Mass-Energy-Economic (RMEE) (pronounced 'army') methodology invented by this research.

The paper presented in Chapter 2 has been accepted for publication in the International Journal of Life Cycle Assessment. The research shows that current methodologies lack the ability to ensure consistent system boundaries are selected when comparing systems for decision making. The RMEE method is presented with an example to demonstrate how it is completed. For an example where the application of RMEE is compared to not applying the method, refer to Appendix I where a LCA of various ethanol sources is presented.

2.1 Introduction

As life-cycle assessment (LCA) becomes a common tool to aid in making business and policy decisions, it is crucial that the methodology become more rigorous and transparent [Total Life-cycle Conference – 1997, 1998][1] [2]. Since decision making and design improvement involves making choices, it is inevitable that LCA will be used to compare alternative systems providing a similar product or service. Good selection/rejection decisions between system options requires that systems be comparable not only in the products or services they provide, and in data quality, but also in the depth of detail included/excluded in each system's analysis. In other words, it is essential to have a rigorous method of deciding which elements, or unit processes, of a system are to be included in an LCA analysis such that a "fair" comparison between systems results. The LCA standards of ISO 14000 recognize this by stating,

"In comparative studies, the equivalence of the systems being compared shall be evaluated before interpreting the results. Systems shall be compared using the same functional unit and equivalent methodological considerations, such as performance, system boundaries, data quality, allocation procedures, decision rules on evaluating inputs and outputs and impact assessment." [3]. (Note: definitions of terms used throughout this paper are provided in the next section)

Because of the importance of system boundary selection (SBS), the ISO standard requires disclosure of the system boundary selection (SBS) method used - "The criteria used in establishing the system boundaries **shall** be identified and justified in the scope of the study." [3].

There are several aspects or "dimensions" involved in selecting system boundaries. System boundary dimensions identified by TILLMAN *et al* [18] are as follows:

- I. boundaries between the technological system and nature,
- II. geographical area,
- III. time horizon,
- IV. production of capital goods,

V. boundaries between the life-cycle system of the studied product (or service) and the connected life-cycle systems of other products.

This work focuses on developing a method to select boundaries of dimension V, between the life-cycle system of the studied product or service and the connected life-cycle systems of inputs to the primary life-cycle system. Because the production of capital goods can be considered a connected life-cycle system, the methodology developed in this paper is also applicable to dimension IV of system boundary selection. Another element of dimension V is the analysis of outputs and how they are included or excluded in the system. Waste outputs often require further, sometimes intensive, downstream processing (e.g. hazardous waste treatment, waste collection/ sorting/ disposal/ monitoring). The question is whether or not these processes or services are systematically included or excluded in the boundary of the life-cycle system. Because these services have a cost associated with them, the method proposed here is equally applicable to answer this question. A second category of outputs requiring system boundary consideration is co-products and by-products. These are products and nonwaste outputs, respectively, which do not contribute to the functional unit of concern [4]. Nonetheless, co-products and by-products share processes in the life-cycle stages of the primary product system, and their contribution (or share of responsibility) needs to be determined and properly allocated. Evaluation of allocation methods is not completed here.

Material and energy inputs within the system boundary of an LCA typically encompass various life-cycle stages including raw materials acquisition, manufacturing, transportation, use/reuse/maintenance, and recycle/waste management [5]. The classical figure, presented by FAVA et al, illustrating these boundaries is shown in Figure 2.1 [5]. The general practice and objective of system boundary selection is summarized by BOGUSKI et al [6]:

"After all the steps that fall within the system boundaries are identified, the practitioner may choose to simplify the LCI or LCA by excluding some steps from the study. This must be done with extreme caution and only after the entire system has been examined. The general rule for excluding steps from the study is that a step may be excluded only if doing so does not change the conclusions of the study."

The major difficulty of this general rule is how does one prove a step will not change the conclusions without first completing the LCA? If one must collect data to prove this, then why exclude the step if the data exists and has been included in the LCA? Furthermore, to test if a particular "step" in the life-cycle affects the conclusions one must have assumed a system boundary to begin with. In short, this rule is not practical for LCA practitioners who must make rigorous comparative decisions with limited time and resources. The Relative Mass-Energy-Economic method for system boundary selection allows the LCA practitioner to select system boundaries and exclude unit processes or "steps" from the study before examining the entire system and to do this in a practical, repeatable and quantitative means.

The three objectives of this paper are:

- 1. to thoroughly review the current practice of system boundary selection in the field of LCA,
- 2. to demonstrate the need for a rigorous method for selecting LCA system boundaries, and
- to present the development of a new system boundary selection (SBS) method called the Relative Mass-Energy-Economic (RMEE) method for system boundary selection.

RMEE is revealed to be practical, repeatable, and quantitative – qualities missing to varying degrees from existing LCA system boundary selection methodologies.

2.1.1 Definition of Terms

For conciseness this paper assumes a certain level of knowledge of LCA methodology. Because the vocabulary of LCA is currently in development and for those readers not as familiar with LCA terms, Table 2.1 below provides definitions of terms used in this paper.

Table 2.1:	Definition	of Terms
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Word	Definition
life-cycle system	The collection of unit processes linked together by materials and energy to provide a function associated with a product or service. E.g. the collection of processes involved in producing ethanol fuel.
functional unit	A common unit of comparison between life-cycle systems. The functional unit may consist of one or a combination of products and services . E.g. for fuel ethanol production systems the common unit of comparison is a specific amount of ethanol, animal feed, and compressed CO_2 captured as a product for resale (often sold to the beverage industry) since all three are products of the life-cycle system.
unit process	An individual component in the system performing an activity within the life- cycle of the final product or process being analyzed. E.g. a corn ethanol conversion plant is a unit process within the entire life-cycle system.
outputs	Marketable products or services from a unit process. These include the primary product and any co-products from a specific unit process.
inputs	Material, energy and service inputs to a unit process.
environmental	Any form of pollution from a unit process, including air emissions, water
outputs	effluents, solid waste, noise, etc
economic value	The market value of a product or service as seen by the consumer. E.g. the cost of automotive fuel at the pump.
capital goods	Machinery, buildings, and all other structures or infrastructure required for the operation of a life-cycle system. Examples include: refineries, roads, and manufacturing plants for the life-cycle system of an automotive fuel.
comparative LCA	A life-cycle assessment making a comparison between at least two different systems for providing a defined functional unit. E.g. if the functional unit is ethanol fuel, a comparative LCA could compare ethanol from corn, ethanol from wheat, and ethanol from poplar trees.
system boundary selection (SBS)	A process required by all LCA studies to decide which unit processes in a system are to be included in the system boundary for environmental analysis.
Relative Mass-	A method of SBS in which the relative mass, energy and economic value of
Energy-Economic	each input to each unit process is compared to the functional unit of the
SBS method	system. This is the method invented and developed by the author in this paper.
cut-off ratio	A value set by the LCA practitioner to decide whether an input is to be included in the system.
unit process	System boundaries are selected by considering the relative mass of inputs
mass percentage method of SBS	to a given unit process and eliminating upstream processes from all inputs contributing less than the defined cut-off ratio. Refer to Figure 2.1.
cumulative mass-	System boundaries are selected by considering the relative mass or energy
energy method of SBS	input of a unit process to the entire system's total mass and energy inputs. Refer to Figure 2.3.



Figure 2.1: General LCA System Boundaries

2.2 Characteristics of Good System Boundary Selection Methodology

In theory, the system describing the entire "cradle-to-grave" life-cycle of a product or process is nearly infinite. One could take a given product system to such detail as to include the entire manufacturing and material extraction for a wheel bolt of a truck transporting office paper to a refinery to produce gasoline, and beyond. Indirectly every product or process is connected within the global economic web. This is not practical for the LCA practitioner (although there is an interesting body of research developing at Carnagie-Mellon University using macro-economic input-output analysis to model the interconnected economy and potential environmental loading)[7].

The ultimate objective of a LCA is to identify and quantify all significant environmental outputs associated with the product or service system. As ISO 14041 states: "Resources need not be expended on the quantification of such inputs and outputs that will not significantly change the overall conclusions of the study."[3]. In practice, the LCA practitioner does not have the resources available to quantify all the environmental outputs of all the unit processes in a system and then identify which unit processes significantly contribute to the overall life-cycle environmental outputs of the desired product. Due to limited time and resources for completing LCA decisions, the practitioner must be able to draw system boundaries without having to first quantify the environmental outputs of any unit processes.

LCA can often be very subjective, potentially resulting in questionable and highly debatable results. As a result, external verification is essential to current LCA practices. One area of debate is often whether or not a comparative LCA is actually making a comparison between life-cycle systems with equivalent resolution of system inputs and outputs [1]. That is, how does one know two competing systems are be compared with equivalent system boundaries? System boundary selection based on qualitative parameters does not allow for repeatability, resulting in questionable results. As a result, the SBS method must be quantitative and repeatable.

As anyone who has completed an LCA knows, it requires significant time and resources to complete a study. Furthermore, the general trend is to streamline LCA methods to allow faster decision making without the need of excessive resources and time. As a result, a good SBS method must also be simple enough to apply and aid in the efforts of streamlining LCA.

Since the objective of an LCA is to calculate the potential environmental impact of a system, the SBS method cannot be based only on the inputs and outputs of a unit process without considering the significance of the role of the unit process in the life-cycle system. The reason for this is a particular input or output to a unit process may be significant to the unit process, but the unit process itself may not be significant to the environmental performance of the whole life-cycle system. If the SBS method decides which inputs should be included in a system based on the unit process alone, then significant to the decision being made about the life-cycle systems. For example, consider a transportation unit process utilizing diesel fuel. The diesel fuel is a significant input to this unit process but it may be insignificant relative to the life-cycle system as a whole.

Ultimately, the selection of the system boundary affects the completeness or scope of the life-cycle system. The system boundary discriminates between what is within the LCA analysis and what is left outside of the LCA. To allow for a fair comparison between systems the goal is to have systems of similar completeness. Furthermore, in general, the more complete a system is, the greater the time and resources required to obtain and analyze data. It is also true that 100% system completeness is not only impossible to achieve but is also not required to make an educated decision between products or services. As a result, a good SBS method should be able to define different levels or measures of completeness to allow for fair comparisons, and the flexibility to complete streamlined or more detailed LCAs. The method developed within this paper aims to provide this.

In summary, to be efficient and provide a repeatable and rigorous comparison between systems, the SBS method must

- 1. be quantitative (i.e. qualitative judgement rules are not adequate),
- 2. not require the quantification of environmental outputs from every unit process in the life-cycle system before system boundary selection,
- be simple and allow for streamlining (i.e. the SBS method must allow for different degrees of rigor due to varying availability of time and resources to make decisions),
- 4. consider the significance of inputs and outputs relative to the system as a whole, not only to an individual unit process,
- 5. provide the ability to define measurable levels of system completeness.

2.3 Current System Boundary Selection Procedures

The ISO 14040 document [8] recognizes different methods of SBS exist, and also the potential shortfall of the mass percentage method –

"There are several criteria that are used in LCA practice to decide which inputs will be studied, including 1)mass, 2)energy, and 3) environmental relevance. Making the initial identification of inputs based on mass contribution alone may result in important inputs being omitted from the study. [8]".

The following discussion reviews the various existing methods of SBS currently being practiced.

Many LCA studies arbitrarily and qualitatively select system boundaries by considering only the "main" life-cycle stream [9][10]. These qualitative methods do not allow for repeatable boundaries to be selected, nor do they ensure similar boundaries are selected for different systems.

Other LCA's have used the percentage of the mass of unit process mass inputs to cut system boundaries which is a first step to a quantitative method of SBS [11]. However, this method considers only the inputs to a given unit process with respect to its self by calculating the percent each input contributes by mass to the total unit process inputs. A cut-off ratio is then chosen. The cut-off ratio is often 0.05 or 0.10 meaning any input contributing less than this ratio is considered insignificant to the unit process and is then not studied further upstream. The major disadvantage of this method is it considers only the relationship of each input to a unit process and not its significance to the entire life-cycle system.

Figure 2.2 illustrates the system boundary selection method by mass percentage of unit process inputs where a cut-off criteria of 0.05 or 0.10 by mass would consider Input C to be insignificant but require upstream analysis of both Input A and Input B. Although Input A and Input B may be significant inputs to Unit Process 101, relative to the system as a whole they may be completely insignificant. As a result, the LCA practitioner may waste substantial time and resources searching for and analyzing data upstream of Inputs A and B which in the end will have no impact or relevance to the end result of the complete system analysis. On the other hand, if Unit Process 101 is near the downstream end-point (i.e. closely linked to the functional unit), Input C could be a significant input to the functional unit. Yet, by considering only the ratio of unit process inputs it would be eliminated from the system with a 0.05 rule.

Obtaining data for a life-cycle assessment is often the most costly step. As a result, many LCA studies choose system boundaries based on what data can be most readily obtained [12]. If data for a particular unit process are considered difficult and costly to obtain, the practitioner might be more easily persuaded to exclude it from the system boundary. The reverse is also true, where simply because the data is available the unit process will be included in the system boundaries. One might claim, by including these unit processes the study is that much more complete and "detailed". Two problems arise from including unit processes only because the data is available:

 A false sense of completeness or detail can be interpreted when unit processes known to be relatively insignificant are included. The audience of the LCA study might interpret this as the entire LCA having been investigated to a similar level of detail. 2) When comparing life-cycle systems for decision making it is necessary that all systems be similarly complete [3]. The addition of unit processes with data to one system may make that particular system more complete, but if similar detail is not added to the other systems the comparison becomes biased.

In short, defining system boundaries based on data availability is an unacceptable method because it is not repeatable, has no scientific justification, and is not rigorous.

The ISO criteria of "environmental relevance" is not practical because it requires one to evaluate the environmental outputs for every unit process in a system before system boundaries can be drawn. In other words, it requires the practitioner to have fully completed the life-cycle inventory before system boundaries are chosen. This does not support streamlining efforts to make LCA more time and resource efficient. Furthermore, it requires an impact assessment to establish the "environmental relevance" of a unit process, however, "environmental relevance" is currently a very qualitative process [1]. This does not allow for repeatability due to the judgements required. Although it would be advantageous to be able to select system boundaries based on the environmental relevance of a unit process, it is not practical because of the difficulty in quantifying in a repeatable manner the environmental relevance of a unit process before having assessed the life-cycle system.

One criteria ISO does not mention is selection by "economic value". Economic value is a very practical criteria for system boundary selection because it captures those inputs which have very little mass or inherent energy yet have substantial upstream process inputs (materials and energy) and associated environmental outputs. An example of these inputs is precious metals such as gold or platinum. These materials in the use of a system often are small in quantity (i.e. low relative mass), are not considered energy inputs, but are very costly to the consumer. They also require a significant amount of resources (materials and energy) to extract and process. The economic value of the precious metals provides a proxy for the extent of the upstream energy and material inputs. Furthermore, as processes result in environmental impacts of significant public concern (toxins, greenhouse gases, acid rain, water pollutants, etc.) the economic cost of managing these

potential environmental impacts become embedded in the product. As a result, economic value is a valid criterion for system boundary selection. However, the current economic value of products tends not to include the cost of externalities. The LCA practitioner must take caution in using the economic criteria for system boundary selection for evaluations of toxic releases or other low quantity but highly environmentally significant outputs.

The ISO methodology concentrates on mass and energy criteria and states the rules for system boundary selection to be:

"1) Mass is an appropriate decision rule, when using mass as a criterion, would require the inclusion in the study of all inputs that cumulatively contribute more than a defined percentage to the mass input of the product system being modeled. 2) Energy similarly, a criterion should be established to require the inclusion in the study those inputs that cumulatively contribute more than a defined percentage of the product system energy inputs." [8]

Theoretically this is a robust method of drawing system boundaries because by considering the total life-cycle mass and energy inputs required to provide a functional unit, one can define a percentage considered significant to include in the study. In other words, if we know the system's grand total of all energy inputs ($E_{System Total}$) and all mass inputs ($M_{System Total}$), it is possible to systematically move upstream from the functional unit and consider each energy and mass input's (E_i and M_i) contribution to the total. This means calculating $E_{i\%} = (E_i / E_{System Total} * 100)$ and $M_{i\%} = (M_i / M_{System Total} * 100)$ and comparing these with the defined "cut-off" ratio. If either $E_{i\%}$ or $M_{i\%}$ is greater than the cut-off ratio then one includes the input and its upstream unit process in the system boundary. The practitioner continues to move upstream (or downstream for handling wastes) until all $E_{i\%}$ and $M_{i\%}$ are less than the cut-off ratio. For example, referring to Figure 2.3, the energy and mass flows E_1 and M_1 (inputs to unit process 1, products of unit process 2) contribute a percentage of the total system energy and mass inputs ($E_{System Total}$, $M_{System Total}$) which is greater than the defined cut-off ratio, hence Unit Process 2 is included in the system boundary. Similarly, unit processes 3, 4, and 5 are included in the

system boundary because the material or energy flows from them (flows M_2 , E_2 , M_3 , E_3 , M_4 , E_4) contribute an energy or mass component to the total which is also greater than the cut-off ratio. Unit processes 6 and 7 are excluded from the LCA analysis because the relative energy or mass contribution of the flows 5 and 6 compared to the total system energy and mass inputs is less than the cut-off ratio.

In practice the suggested ISO method is not practical. The ISO cumulative mass-energy method of system boundary selection is impractical due to the need to calculate the grand totals of a system ($E_{System Total}$ and $M_{System Total}$). In theory the grand total of energy or mass involves the infinite sum of smaller and smaller contributions to the system. In order to calculate the total one must first make an implicit larger system boundary. How does one choose this initial larger boundary to calculate the totals? It is simply not practical, if at all possible, for the LCA practitioner to attempt to calculate the total mass and energy inputs of any given system. In short, the ISO method of system boundary selection is rigorous and robust in theory, but in practice fails.

Another methodology, presented by BESNAINOU and COULON [13], agrees with the ISO methodology that the mass criteria is not adequate for system boundary selection:

"So far, weight has been used as the sole cutoff criterion since this information is always available...This is not satisfactory, however, and a set of cutoff criteria should be used instead of a single criterion.".

In response, their methodology defines four criteria for system boundary selection:

- 1. weight,
- 2. energy requirement,
- 3. toxicity (either of the component itself or due to its manufacturing process), and
- 4. price.

These four criteria are used to qualitatively categorize components to the system to have either a "negligible contribution", "small contribution", or "large contribution" [13]. Although this method has defined important criterion and appears to consider the system as a whole, it remains unrepeatable due to its qualitative nature.



Figure 2.2: SBS by Mass Percentage of Unit Process Inputs



Figure 2.3: Cumulative Mass-Energy Method of System Boundary Selection

Table 2.2 lists a number of LCA studies and the method of system boundary selection chosen. None of which the author considers rigorous enough for current LCA work because they are not quantitative. These methods rely heavily on the knowledge and professional experience of the practitioner. As a result, the need exists for a SBS method which is practical, repeatable, rigorous, and robust.

Authors (Year)	Quote from System Boundary Selection Section of Report	SBS Method	Source
Mann, M.K.; Spath, P.L.; Craig, K.R. (1996)	"Very often, the determination of system boundaries is made based on data availability, and to a large extent, this is how the present analysis was conducted."	Data Availability	[12]
Vigon, B.; Tolle, D.; Evers, P.; Freeman, S.; Landucci, R. (1996)	"general material flow diagrams were constructed focusing on the most important environmental considerations at each stage of the life-cycle"	Qualitative Environmental Relevance	[14]
Hocking, M. B. (1994)	No specific system boundary selection method provided.	Qualitative with consideration of relative energy use.	[9]
Hunt, R.G.; Sellers, J.D.; Franklin, W.E. (1992)	"Second-tier impacts must be investigated, but if in aggregate all of the second-and third-tier operations contribute less than 5 percent to the total, they are excluded from the study."	Set percentage of mass to total.	[11]
Deloite & Touche (1991)	No specific system boundary selection method provided.	Qualitative, non- specified.	[10]
Tyson, K.S.; Riley, C.J.; Humphreys, K.K. (1993)	"We examined a number of previous studies to determine the effect of excluding pre- and post-operational phases." – The study included "Only the operational phase of a fuel cycle"	Energy percentage cut-off based on other studies.	[15]

 Table 2.2:
 System Boundary Selection (SBS) Methods of Various LCA Studies

2.4 The Relative Mass-Energy-Economic (RMEE) Method of System Boundary Selection

The SBS method presented below is a systematic method allowing the LCA practitioner to work upstream from the unit process providing the functional unit. As the LCA practitioner moves upstream a decision is made whether or not each unit process providing a product or service is to be included in the system boundary. This method has been termed the Relative Mass-Energy-Economic (RMEE) method for SBS. RMEE is pronounced "army".

2.4.1 RMEE Step-by-Step

Defining Parameters for System Boundary Selection

System boundary selection by means of a relative ratio remains or continues to be the easiest means of determining whether or not a given unit process should be considered within the system boundary or not. The question is, "ratio of what?". The ratio applied must act as a proxy for the potential upstream environmental impact of providing a given product or service.

As discussed previously, mass ratio has been used in the past to compare the relative contribution of inputs to a given unit process. Mass as a proxy for potential upstream environmental impact due to the production of a product is valid because products with significant mass require transportation, processing, and extraction of raw materials. These processes require energy and can result in significant combustion related air emissions. However, on its own, relative mass is inadequate because many inputs with significant upstream environmental outputs can have little or no mass, such as natural gas or electricity. These are significant energy inputs.

As a result, relative energy contribution must also be considered in selecting system boundaries. Energy content (measured by heating value) of a product as a proxy for potential upstream combustion related air emissions is valid because the production, distribution, and extraction of raw materials to provide energy can result in significant upstream emissions.

In addition to mass and energy, the RMEE method uses economic value as a third parameter for determining whether or not to include a unit process. Economic value is an important criteria for capturing those inputs with little mass or energy value but do have significant upstream energy inputs and related combustion emissions. Upstream processes that are energy or material intensive often produce costly products or services. The economic criterion identifies these processes. For example, precious metals as an input to a manufacturing process (or a product such as an automobile) would have a low percentage contribution by mass or energy, but could have a significant economic contribution. The production of precious metals is very material and energy intensive and should often be included in the system boundaries.

The RMEE method has been developed with energy and manufacturing systems in mind with a primary interest in air emissions resulting from combustion processes. For this focus, mass, energy, and economic value are valid proxies for potential upstream emissions of products. However, for LCA comparisons concerned primarily with toxic releases, additional parameters (e.g. toxicity of materials) may be required. These additional parameters would be designed to ensure products with a relative low mass, low energy value, and low cost but high upstream releases of toxins, are included in the analysis.

As the cost of monitoring, handling and managing hazardous and toxic substances increases, the economic criteria will better capture these and require inclusion of these unit processes in the system. In certain jurisdictions the cost of hazardous material management will not be reflected in the price of the service or product and could result in exclusion of a number of "small" unit processes which together may result in significant toxic releases. Because current economic systems tend not to capture the external costs associated with toxic releases, the RMEE method is not recommended for LCA studies wishing to quantify toxic outputs. In the future, should external costs be better captured, RMEE may be more appropriate for analyzing LCA systems with toxic emissions. However, in its current form, RMEE is limited to energy and product life-cycle assessments where the decision maker's primary interest is in common combustion related air emissions such as carbon dioxide, hydrocarbons, nitrogen oxides, and sulphur oxides.

Similar to work by BESNAINOU and COULON [13], RMEE uses mass, energy and economic value as criteria for system boundary selection. In the method presented by [13] it is not clear how "negligible, small, and large contribution" is determined. Nor is it clear whether or not one must first identify all the components of the system before one can begin the method for system boundary selection. The Relative Mass-Energy-Economic method presented here attempts to clarify this with a quantitative, repeatable, and systematic method for defining the "contribution" of an input to the whole system.

Defining the Ratio for System Boundary Selection

The "contribution" considered by RMEE is the relative contribution of mass, energy or economic value to the defined functional unit. In other words, each input is compared by mass, energy and economic value to the total mass, energy value and economic value of the functional unit. This allows the practitioner to clearly define a ratio to be used to decide whether or not an upstream unit process will be included in the system boundary or not. The lower the ratio, the larger the system boundary, and the more detail included in the study. Because comparative systems share the same functional unit, this also allows appropriate comparison between systems. Comparable boundaries between systems are ensured by declaring the system boundaries to include all those unit processes providing products or services which contribute a given amount to the functional unit by mass, energy or economic value. The result is a quantified system boundary, which can be repeated for different systems in a comparative LCA.

The Steps to Complete RMEE System Boundary Selection

The steps for the RMEE method are as follows:

1. Identify and define the functional unit for the LCA;

- Calculate the total mass, energy, and market economic value of the functional unit, define these as: M_{Total}, E_{Total} and \$_{Total} respectively¹;
- Define a system boundary "cut-off" ratio (Z_{RMEE}). One might initially define Z_{RMEE} as 0.20, complete the life-cycle inventory and decide whether or not more detail is required to make a comparison. If a more detailed comparison is considered necessary, Z_{RMEE} is lowered and the results considered again. (Refer to Table 2.9)
- 4. Begin at the unit process closest to the functional unit, with inputs a, b, c, ..etc.. Quantify the mass (M_i), energy (E_i) and economic value (\$_i) of each input (i=a,b,c). Inputs without a meaningful mass or energy value are assigned zero (e.g. electricity is assigned zero for mass, while most process chemicals are assigned zero for energy since their purpose is not an energy input). Document the sources of data, calculations, and assumptions made.
- Calculate M_{Ratio} = M_i/M_{Total}, E_{Ratio} = E_i/E_{Total}, and \$_{Ratio} = \$_i/\$_{Total}. This defines the relative contribution of each input by mass, energy and economic value to the functional unit.
- 6. If M_{Ratio}, E_{Ratio}, or \$_{Ratio} is greater than Z_{RMEE}, then the upstream unit process of this input is to be included in the system boundary. If neither M_{Ratio}, E_{Ratio}, nor \$_{Ratio} is greater than Z_{RMEE}, then the input is considered "cut-off" and its unit processes upstream from it are not included in the system boundary.
- Repeat the process for each input of all unit processes included in the system, until all inputs are "cut-off".

The procedure is shown in Figure 2.4.

The RMEE method is also used to consider inputs from capital equipment and maintenance by considering the lifetime of capital equipment and frequency of maintenance compared to the needs of the functional unit. The primary advantage of the RMEE method for system boundary selection is, by defining a specified cut-off ratio, independent LCA practitioners can select similar system boundaries for independent analysis.

¹ The market value of any product or service is a fluid value due to changes in the economy. However, LCA generally takes a "snap-shot" in time of a system for analysis, as a result a current static value should



Figure 2.4: The RMEE Method of Life-cycle System Boundary Selection for LCA Purposes

be used for the market value of products or services for the RMEE method.

2.4.2 The RMEE System Boundary Selection Method Demonstrated

The RMEE method is demonstrated for a life-cycle system of the production of ethanol from corn. This example is intended to demonstrate RMEE and should not be considered a complete LCA of ethanol fuel. (For a complete comparison between sources of ethanol fuel refer to [17]). Figure 2.5 shows a relatively detailed system for the production of ethanol. The entire system could have been the boundary selected; a relatively arbitrary boundary. There is no indication or measure of how complete the system boundary is at this point, nor if upstream unit processes have been "cut-off" at equivalent points.

Consider the RMEE technique for system boundary selection. Assume we are beginning the LCA and have defined the functional unit to be the products from the corn ethanol plant: ethanol, distillers dried grains and solubles (DDGS) (used as cattle feed), and carbon dioxide for the beverage industry. Following the steps described above:

Step One: Define the Functional Unit

The functional unit is defined as 150 million liters of ethanol, 127,000 tonnes of distillers dried grains and solubles (DDGS), and 97,000 tonnes of carbon dioxide. These are the annual production rates for the given corn ethanol plant [17].

<u>Step Two</u>: Calculate the Total Mass, Energy and Economic Value of the Functional Unit

Table 2.3:Calculation of Mass, Energy and Total Economic Value of the
Functional Unit

Product	Mass (kg)	Energy (MJ)	Economic Value (\$)
Ethanol	1.19E+08	3.18E+09	\$49.5 Million
DDGS	1.27E+08	1.91E+09	\$27.9 Million
CO ₂	9.70E+07	0.00E+00	\$9.7 Million
Totals:	M _{Total} = 3.43E+08	E _{Total} = 5.08E+09	\$Total = \$87.1 Million

Note: The values used in this table have been obtained from a study being completed comparing different sources of ethanol fuel by Raynolds et al[17].

Step Three: Define a System Boundary "Cut-Off" Ratio

For a first iteration, the cut-off ratio (Z_{RMEE}) will be defined as 0.20. (The results of Z_{RMEE} set at 0.10 and 0.05 will also be shown for comparison.)

<u>Step Four</u>: Quantify the Mass, Energy and Economic Value of Each Input to the Current Unit Process

The current unit process under investigation is the one closest to or producing the functional unit: "Corn Ethanol Conversion". Table 2.4 lists and quantifies the mass, energy and economic value of each input to the corn ethanol conversion plant. For the purpose of reporting, document the sources of data, calculations, and assumptions made.

Table 2.4:Mass, Energy and Economic Value of Inputs to the Ethanol
Conversion Unit Process for Producing the Functional Unit

Input (i)	Mass (M _i) (kg)	Energy (E _i) (MJ)	Economic Value (1998) (\$ _i) (\$)
Corn	3.80E+08	5.51E+09	\$44.8 Million
Natural Gas	8.94E+09	2.64E+09	\$7.50 Million
Electricity	n/a	7.20E+06	\$90,000
Chemicals (Total)	2.08E+06	n/a	\$6.00 Million
Sodium hydroxide	8.40E+05	n/a	no data
Sulphuric Acid	4.00E+05	n/a	no data
Ammonia	8.40E+05	n/a	no data
Water	2.20E+09	n/a	\$0.00
Enzymes (Total)	6.30E+05	n/a	\$1.00 Million
Enzyme - alpha- amylase	1.30E+05	n/a	no data
Enzyme - gluso- amylase	5.00E+05	n/a	no data
Maintenance	n/a	n/a	\$1.00 Million
Construct Plant	no data	no data	\$5.10 Million

Note: Values are based on the inputs required to provide the functional unit. These values have been obtained from a study being completed comparing different sources of ethanol fuel[17]. 1. – Values for "Construct Plant" are distributed over a 30 year life span.

n/a = not applicable

<u>Step Five</u>: Calculate Relative Contribution of Each Input to the Functional Unit Totals

Input (i)	M _{Ratio} (=M _i / M _{Total})	E _{Ratio} (=E; / E _{Total})	\$ _{Ratio} (=\$ _i / \$ _{Total})
Corn	1.10	1.08	0.51
Natural Gas	26.06	0.52	0.086
Electricity	n/a	0.001	0.001
Chemicals (Total)	0.01	n/a	0.06
Sodium hydroxide	0.002	n/a	< 0.06
Sulphuric Acid	0.001	n/a	< 0.06
Ammonia	0.002	n/a	< 0.06
Water	6.41	n/a	0.00
Enzymes (Total)	0.002	n/a	0.01
Enzyme - alpha- amylase	0.000	n/a	< 0.01
Enzyme - gluso- amylase	0.002	n/a	< 0.01
Maintenance	n/a	n/a	0.01
Construct Ethanol Plant	no data	no data	0.051

 Table 2.5:
 Relative Mass, Energy, Economic Value of Each Input

Note: Values in bold are all those greater than 0.20

Note: Values may be greater than 1 due to efficiency in energy or mass transfer to the functional unit. i.e. Most systems will require significantly more energy inputs than the energy value of the final system products or services.

<u>Step Six</u>: Select those Inputs With Relative Mass, Energy, or Economic Value Greater Than Cut-Off Ratio

By comparing the relative mass, energy and economic values from Table 2.5, with the system boundary cut-off ratio (Z_{RMEE}), defined here as 0.20, 0.10 and 0.05, select all inputs with either M_{Ratio} , E_{Ratio} , or S_{Ratio} greater than 0.20. This results in the inputs shown in Table 2.6 to be followed upstream to their associated unit processes.

For Z _{RMEE} = 0.20	For Z _{RMEE} = 0.10	For Z _{RMEE} = 0.05
Corn	Corn	Corn
Natural Gas	Natural Gas	Natural Gas
Water	Water	Water
		Chemicals (Total)
······································		Construct Ethanol Plant

 Table 2.6:
 Inputs to be Followed Upstream

In this case, for both 0.10 and 0.20 cut-off ratios the same inputs are to be followed upstream. Only at a Z_{RMEE} value of 0.05 is increased detail required.
Step Seven: Move to Next Upstream Unit Process

For the 0.20 cut-off ratio the next tier of unit processes to consider are:

Transport Corn Transport Natural Gas Supply Water

For the purpose of demonstration only the corn stream is followed through.

Transport Corn

The inputs to the unit process "Transport Corn" includes the corn itself, diesel fuel, the truck, and maintenance of the truck. Using the RMEE method using Z_{RMEE} equal to 0.20, the only input to be further investigated upstream from "Transport Corn" is corn, as seen in Table 2.7 below.

Input (i)	M _{Ratio} (=M _i / M _{Total})	E _{Ratio} (=E _i / E _{Total})	\$ _{Ratio} (=\$ _i / \$ _{Total})	
Corn	1.11	1.08	0.51	
Diesel Fuel	0.002	0.01	0.004	
Truck Maintenance	n/a	n/a	0	
Capital – Truck	0	n/a	0	

 Table 2.7:
 Relative Mass-Energy and Economics for Transport Corn

Produce Corn

Table 2.8 shows the relative contribution of each input of producing corn compared to the functional unit.

rable 2.0. Relative Mass-Energy and Economics for Corn riouwerion							
Input (i)	M _{Ratio} (=M _i / M _{Total})	E _{Ratio} (=E _i / E _{Total})	\$ _{Ratio} (=\$ _i / \$ _{Total})				
Land drainage	n/a	n/a	0.004				
Machinery repairs	n/a	n/a	0.03				
Building repairs	n/a	n/a	0.005				
Fertilizer - N	0.02	n/a	0.075				
Fertilizer - K2O	0.0078	n/a	0.02				
Fertilizer - P2O5	0.01	n/a	0.02				
Crop protectants	no data - low quantity	n/a	0.05				
Seed	no data - low quantity	n/a	0.05				
Diesel	0.002	0.003	0.0038				
Propane	0.02	0.06	0.0036				

 Table 2.8:
 Relative Mass-Energy and Economics for Corn Production

As the above table shows, all inputs are "cut-off" for a cut-off ratio of 0.20 and 0.10. When the cut-off ratio is lowered to 0.05, nitrogen fertilizer, crop protectants, and seed are followed upstream to their unit process source.

The final system boundaries with a 0.20, 0.10, and 0.05 cut-off ratio are shown in Figure 2.5. It is only fortuitous and case specific that 0.10 and 0.20 boundaries are the same.

For an example of RMEE used in defining the system boundaries for an LCA comparing three sources of ethanol fuel, refer to [17].

2.4.3 Selecting the RMEE Cut-off Ratio (Z_{RMEE})

Up to this point the RMEE method for system boundary selection has provided a systematic and quantitative means to consistently select system boundaries based on a given cut-off ratio. In other words, with a specified cut-off ratio (Z_{RMEE}), different LCA practitioners can complete an analysis on similar systems providing the same functional unit and expect to obtain consistent depth in system boundaries.

However, how does one select an appropriate cut-off? The lower the Z_{RMEE} the more expanded the system boundaries are, and the more detailed data collection must be to complete the LCA. Appropriate selection of the cut-off ratio depends on the objective of the LCA, the resources available to complete the LCA, and the data sources available. A largely funded academic study with access to detailed industry data may select a cut-off ratio of less than 0.01 to provide a detailed study. However, in general, no specific cut-off ratio can be prescribed for all LCA studies.

From experience of applying RMEE in industry and published work [17], Table 2.9 presents three different cut-off ratios and their general appropriateness of use.

Table 2.9:	Selecting a RMEE Cut-off Ratio (Z _{RMEE}): Author experience based
	generalizations

RMEE Cut-off Ratio		General Description	Appropriate Use		
0.20		Generally captures only the primary energy, material, and cost inputs to the system. Typically eliminates need to investigate	High-level comparisons of systems, compiling preliminary results, identifying primary unit processes for design		
		most unit processes of capital construction (e.g. buildings for a facility, etc.) and ancillary materials.	improvement.		
. 0.10		Requires enough detail to include significant ancillary inputs. Allows practitioner to investigate and understand the implications of more detailed design improvements.	Internal corporate decision making and overall design improvement.		
0.05	0	Provides a very detailed analysis often including the cost and environmental implications of construction and decommissioning facilities.	Public claims for superiority of one system over another, assessing systems for environmental output credits,		
		Requires substantial resources to complete the life-cycle inventory.	detailed engineering design improvements.		

A more scientific means of deriving the relationship between the cut-off ratio (Z_{RMEE}) and uncertainty in the results of an LCA is presented in Part 2 of this paper "Part 2: Selecting the Boundary Cut-off Parameter (Z_{RMEE}) and its Relationship to Overall Uncertainty".

2.5 Conclusions

Based on the authors review, existing methods of selecting system boundaries do not adequately meet the needs of current LCA practice that is quantitative, repeatable, and streamlined. The system boundary selection methodology developed here by the author, called the Relative Mass-Energy-Economic (RMEE) method, is a quantitative means of consistently drawing comparable system boundaries for systems being compared in an LCA. Because RMEE requires only knowledge of material input and output streams (not environmental data which is most time intensive) and begins furthest downstream working upstream systematically, it is far more time and resource efficient than other system boundary selection methods. The primary difference of the RMEE method compared to other methods of system boundary selection is that RMEE defines the boundary based on the relative mass, energy and economic value of inputs to unit processes compared to the mass, energy and economic value of the functional unit of the LCA. This leads to a more repeatable method for system boundary selection in LCA and helps ensure comparable boundaries are set for different systems providing the same functional unit.

The RMEE method is particularly well suited for LCA studies comparing energy or product systems based on common combustion related air emissions. The RMEE method is not considered suitable for studies primarily concerned with toxicity because the mass, energy, and economic criteria for inputs do not necessarily capture unit processes with toxic releases to the environment.

In short, RMEE:

- Allows for a fair comparison of different systems providing the same functional unit.
- Quantitatively defines system boundaries making it repeatable.
- Is simple to calculate, requiring only material, energy and service input and output data for those unit processes that will end up in the system boundary. In other words, time and resources are not wasted collecting or estimating environmental data for unit processes not included in the system boundary.
- Produces input and output data that is required for the inventory analysis. Once RMEE is completed, the material, energy and service flows within the system boundary have been quantified, completing a significant portion of the inventory analysis.
- Can be used to determine if capital equipment should be included in the system boundary. The method is not limited to products, services can be considered as well.
- Is designed primarily for evaluation of energy and product systems based on common combustion air emissions.

One current shortfall of the RMEE method is the arbitrary selection of the cut-off ratio (Z_{RMEE}) . Further research is being completed to quantify the degree of uncertainty associated with different cut-off ratios. Results of this research are presented in Part 2 of this paper. The results enable RMEE to move the "art" of system boundary selection to more of a "science".



Notes: DDGS = Distillers Dried Grains and Solubles (animal feed); CO2 is compressed and sold to the beverage industry, i.e. it is a product not an emission;

Figure 2.5: LCA System for Ethanol Fuel Production

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Chapter 3

The Relative Mass-Energy-Economic (RMEE) Method for Life-Cycle Assessment (LCA) System Boundary Selection

Part 2: Selecting the Boundary Cut-off Parameter (Z_{RMEE}) and its Relationship to Overall Uncertainty

As concluded in Chapter 2, a method is required for selecting the RMEE system boundary cut-off parameter (Z_{RMEE} Cut-off Ratio) and calculating the uncertainty associated with system boundary selection. Chapter 3 presents the results of modeling over 800 random systems to derive a relationship between the Z_{RMEE} and system boundary uncertainty. From this, the RMEE method for system boundary selection provides a quantitative method of estimating uncertainty in results due to system boundary selection and combining this uncertainty with data uncertainty. Also included is a method of quantifying the probability the mean environmental outputs of one system are less than a competing system. This chapter begins by re-introducing the steps of RMEE.

Chapter 3 is a paper which has been accepted for publication in the International Journal of Life-Cycle Assessment in a slightly shortened version, but is left here in full length to provide additional explanation.

3.1 Introduction

Life Cycle Assessment (LCA) used as an aid to decision making compares service or product alternatives based on their life-cycle economic costs and/or potential environmental impacts. A key step in any life-cycle assessment is to break each alternative into a collection of unit processes representing the life-cycle system. In theory, each system is a collection of hundreds of thousands of unit processes. That is, one could argue any service or product is interconnected with the entire economy. To be of practical use, LCA must draw system boundaries and exclude certain unit processes from its analysis. To make a fair comparison between alternative products or services, one must ensure **similar** boundaries are selected for each system. The first question is "how does one select 'similar' system boundaries? The second important question is, "what effect does the selection of my system boundary have on the uncertainty in my results"?

An answer to the first question, "how does one select similar system boundaries?", is provided by the related paper which presented "The Relative Mass-Energy-Economic (RMEE) Method of System Boundary Selection – A Means to Systematically and Quantitatively Select LCA Boundaries – Part 1"[1]. The current paper, Part 2, focuses on the second question, "what effect does system boundary selection have on the uncertainty in the results of an LCA?". Therefore, the <u>objective</u> is to quantify the relationship between the system boundary cut-off parameter (Z_{RMEE}) in the RMEE method and the boundary-related uncertainty in the final results of an LCA.

For a review of the existing methods for system boundary selection and a discussion on the requirements of a useful and rigorous method refer to Part 1 [1] which includes a detailed description, justification, and example of the RMEE method. The present paper briefly describes the RMEE method and provides a simple example, but focuses on developing the relationship between the RMEE system boundary cut-off parameter (Z_{RMEE}) and the uncertainty in the overall results of an LCA due to system boundary selection. The relationship between Z_{RMEE} and uncertainty is presented graphically and in tabular form for further application. Finally, the implications of the RMEE method for system boundary selection are shown through an example comparison of two systems. This example demonstrates how the mean environmental output of one system can be compared to the mean of a competing system to calculate a confidence one system outperforms another.

3.2 The Relative Mass-Energy-Economic (RMEE) Method

What makes the RMEE method different from other methods of system boundary selection is that it is based on examining the ratio between inputs to a unit process and the functional unit. In other words, the method considers each input and asks "How relevant is this input to the functional unit?". If the input is considered significant to the functional unit, then the upstream unit process providing the input is included inside the system boundary of the LCA. If the input is considered insignificant to the functional unit, the upstream unit processes providing the input are "cut-off", that is they are considered outside the system boundary of the LCA. In the RMEE boundary selection method, "significance" is defined by whether the ratio of the input to the functional unit exceeds a chosen value called the Z_{RMEE} cut-off ratio. If the ratio of input to the functional unit is greater or equal to the Z_{RMEE} cut-off, then the upstream unit process is included in the system boundary. If the ratio is less than Z_{RMEE}, the upstream unit processes are excluded from the system boundary. Comparison between the input and Z_{RMEE} is made using three ratios: mass, energy, and economic value. As a result, the mass value of each input is compared to the mass of the functional unit, the energy content of each input is compared to the energy content of the functional unit, and the market value of each input is compared to the market value of the functional unit. If any of the three ratios is greater than the Z_{RMEE} cut-off then the upstream unit processes are included in the system boundary. In the end, the RMEE method provides a repeatable and quantitative method of selecting system boundaries for LCA studies comparing energy or product systems with primary interest in combustion related air emissions.

Extracted from [1] the steps to apply RMEE are as follows:

1. Identify and define the functional unit for the LCA.

- Calculate the total mass, energy, and market economic value of the functional unit. Define these as: M_{Total}, E_{Total} and \$_{Total} respectively¹.
- 3. Define a system boundary "cut-off" ratio (Z_{RMEE}). (Selection of an appropriate Z_{RMEE} is the subject of the remainder of this paper).
- 4. Begin at the unit process closest to the functional unit, with inputs a, b, c, ...etc... Quantify the mass (M_i), energy (E_i) and economic value (\$_i) of each input (i=a,b,c, ...). Inputs without a meaningful mass or energy value are assigned zero (e.g. electricity is assigned zero for mass, while most process chemicals are assigned zero for energy since their purpose is not an input to energy). Document the sources of data, calculations, and assumptions made.
- 5. Calculate $M_{Ratio} = M_i/M_{Total}$, $E_{Ratio} = E_i/E_{Total}$, and $R_{Ratio} = S_i/S_{Total}$. This defines the relative contribution of each input by mass, energy and economic value to the functional unit.
- 6. If M_{Ratio}, E_{Ratio}, or S_{Ratio} is greater or equal to Z_{RMEE}, then the upstream unit process which provides this input is to be included in the system boundary. If neither M_{Ratio}, E_{Ratio}, nor S_{Ratio} is greater than Z_{RMEE}, then the input is considered "cut-off" and the upstream unit processes supplying it are not included in the system boundary.
- 7. Repeat the process for each input of all unit processes included in the system, until all inputs are "cut-off".

The procedure is shown in Figure 3.1 below.

¹ The market value of any product or service may fluctuate due to changes in the economy. However, LCA analysis is generally based on a time and technology "snapshot" of a system. A current static value should be used for the market value of products or services for the RMEE method. When using LCA to assess future projects it is appropriate to use the values generated through an economic analysis of the project.



Figure 3.1: The RMEE Method of Life Cycle System Boundary Selection for LCA
[1]

As a simple example to demonstrate how RMEE is completed, consider System A shown in Figure 3.2, with the data for the flows between unit processes shown in Table 3.1.



Notes: P_i = Product or service e.g. steel, power, etc. from unit process "i". x_i = environmental output from unit process "i".

Figure 3.2: Sample Process Flow Diagram to Demonstrate RMEE: "System A"

Product	Units	Mass (kg / unit)	Energy Content (kJ / unit)	Market Value (\$ / unit)
P _{Fn}	kg	1	10,000	10
P ₂	kg	1	5,000	3
P ₃	kg	1	12,000	18
P.4	kg	1	15,000	2
P ₅	kg	1	9,000	0.75
P ₆	kg	1	3,500	1.5

Table 3.1: Flow Data for System A

Note: For simplicity all flows in this system are materials, i.e. they have a mass, however it is reasonable to expect services or other products which have no mass, e.g. electricity, design services, etc.

Assume the functional unit is defined as 100 units of flow P_{Fn} , and Table 3.2 presents the amount of each flow required to produce the functional unit. Table 3.2 also reports the mass, energy and economic values for each flow based on the data in Table 3.1.

Flow	Amount in	Units	Total Mass	Total Energy	Total Market
1.0.0	System	Сша	in System	in System	Value
	System		•		
			(kg)	(kJ)	(\$)
P _{Fn}	100	kg	100	1,000,000	1000
P ₂	150	kg	150	750,000	450
P ₃	8	kg	8	96,000	144
P4	120	kg	120	1,800,000	240
P ₅	24	kg	24	216,000	18
P ₆	9	kg	9	31,500	13.5

 Table 3.2:
 Flows in System A to Produce the Functional Unit

Table 3.3 presents the calculated ratios M_{Ratio}, E_{Ratio}, and S_{Ratio} for each flow in System A.

Table 3.3:The Mass, Energy and Economic Ratio of Each Flow in System A to
the Functional Unit

Flow	$M_{Ratio} = M_i / M_{Total}$	$E_{Ratio} = E_i / E_{Total}$	$S_{Ratio} = S_i / S_{Total}$
P ₂	1.50	0.75	0.45
P ₃	0.08	0.096	0.14
P4	1.20	1.80	0.24
P5	0.24	0.23	0.019
P ₆	0.09	0.03	0.014

Note: The bold number is the largest ratio of the three (M_{Ratio} , E_{Ratio} , S_{Ratio}) and determines at which Z_{RMEE} ratio the flow is "cut" from the LCA system. For example, the largest ratio for P₂ is the mass ratio (1.50) therefore flow P₂ will not be cut from the system unless the Z_{RMEE} ratio is greater than 1.50.

Based on the results shown in Table 3.3 it is possible to apply different Z_{RMEE} ratios and shift the system boundary. Table 3.4 illustrates for different Z_{RMEE} ratios whether each unit processes is within the system boundary and therefore considered in the LCA, or if it is considered outside the system boundary. Figures 3.3, 3.4, and 3.5 illustrate the system boundary of System A which results from different Z_{RMEE} values.

Z _{RMEE}	UP1	UP2	UP3	UP4		UP6	Diagram
0.05	inside	inside	inside	inside	inside	inside	Figure 3.2
		(M _{Ratio} > 0.05)	(\$ _{Ratio} > 0.05)	(E _{Ratio} > 0.05)	(M _{Ratio} > 0.05)	(M _{Ratio} > 0.05)	
0.10	inside	inside	inside	inside	inside	outside	Figure 3.3
		(M _{Ratio} > 0.10)	(\$ _{Ratio} > 0.10)	(E _{Ratio} > 0.10)	(M _{Ratio} > 0.10)	(M _{Ratio} < 0.10)	
0.15	inside	inside	outside	inside	inside		Figure 3.4
		(M _{Ratio} > 0.15)	(\$ _{Ratio} < 0.15)	(E _{Ratio} > 0.15)	(M _{Ratio} > 0.15)		
0.20	inside	inside		inside	inside		Figure 3.4
		(M _{Ratio} > 0.20)		(E _{Ratio} > 0.20)	(M _{Ratio} > 0.20)		
0.25	inside	inside		inside	outside		Figure 3.5
		(M _{Ratio} > 0.25)		(E _{Ratio} > 0.25)	(M _{Ratio} < 0.25)		

 Table 3.4:
 Application of Different Z_{RMEE} Cut-offs to System A

Note: "inside" = the unit process and its associated environmental impacts are inside the system boundary of the LCA; "outside" = the unit process is outside the system boundary for the given Z_{RMEE} and its environmental impacts are not included in the results of the LCA.



Figure 3.3: System Boundary for System A with Z_{RMEE} set at 0.10



Figure 3.4: System Boundary for System A with Z_{RMEE} set at 0.15 or 0.20



Figure 3.5: System Boundary for System A with Z_{RMEE} set at 0.25

The end result of the RMEE system boundary method for any LCA system is a quantified system boundary determined by the chosen Z_{RMEE} ratio. Two or more systems, which provide the same functional unit and with the same Z_{RMEE} cut-off can then be compared because they have similar system boundaries. The questions not answered by RAYNOLDS et al in Part 1 [1] were: "How does one select Z_{RMEE} ?" and "What degree of uncertainty does the system boundary selection introduce to the overall results?". The remainder of this paper presents answers to these two questions.

3.3 Selecting the Appropriate Z_{RMEE} Cut-off Ratio for RMEE

As shown in the example above for System A, the Z_{RMEE} cut-off defines the system boundary of an LCA. With a smaller Z_{RMEE} ratio, the system to analyze becomes larger. As Z_{RMEE} gets larger, more unit processes are left out of the system, resulting in a smaller analysis problem but more uncertainty as to the 'real' environmental performance of a system. To be able to use LCA for decision making it is important to understand the uncertainty in the results [2][3].

3.3.1 Method to Derive a Relationship Between Z_{RMEE} Cut-off and Uncertainty Introduced into LCA Due to System Boundary Selection

As the Z_{RMEE} cut-off ratio increases, the boundaries decrease and a greater amount of environmental outputs is not included in the final LCA results. At $Z_{RMEE} = 0$ the entire theoretical system is analyzed and accounts for all environmental outputs. In other words, as Z_{RMEE} increases, the fraction of the true total environmental outputs measured by the LCA decreases. At $Z_{RMEE} > 0$, not all unit processes are accounted for and therefore the true total of environmental outputs is not measured.

To find the relationship between Z_{RMEE} and the fraction of total environmental output a stochastic modeling study was completed. Eight-hundred random LCA systems were generated and evaluated at different Z_{RMEE} values using a LCA software package developed by the principal author [see Appendix II for more details on the software]. Each system was randomly generated using rules to generate a realistic distribution of mass, energy and economic inputs throughout the system. Four different types of systems were evaluated, each type defined by the nature of the functional unit produced (refer to Table 3.5). Within each type of system, systems with 50 and 100 unit processes were used. The assumption was made that these systems of 50 and 100 unit processes represent the true total system. The method for generating random systems is described below.

Random System Generation

The type of functional unit provided defines each type of system, described in Table 3.5. Type I is a product with a relatively high heating value (25,000 kJ/kg) and is relatively expensive for a fuel (1 \$/kg). Type II is a lower cost fuel (0.25 \$/kg) with a relatively high heating value (25,000 kJ/kg). Type III is a product with low heating value (5,000 kJ/kg) and medium cost associated with it (100 \$/kg). An example of a Type III product might be a manufactured component or part. Finally, Type IV describes a functional unit with a low heating value (5,000 kJ/kg) but a high cost (1000 \$/kg). Throughout the remainder of this paper each system type will be referred to by the nomenclature defined in Table 3.5.

System Type Number	Type of Functional Unit	Mass per unit of functional unit (kg/unit)	Energy per unit of functional unit (kJ/unit)	Market value per unit of functional unit (\$/ unit)	Example	Nomenclature (Mass, Energy, Market Value)
I	Relatively expensive, high energy value.	1	25,000	1	High value fuel or material with higher energy value e.g. plastics.	(1,25000,1)
II	Relatively low cost, high energy value.	1	25,000	0.25	Low cost fuel, e.g. gasoline, ethanol.	(1,25000,0.25)
III	Medium cost, low energy	1	5,000	100	Medium cost finished product or expensive material. e.g. automotive part	(1,5000,100)
IV	High cost, low energy,.	1	5,000	1000	High market value finished product. e.g. electronics components.	(1,5000,1000)

 Table 3.5:
 The Four Types of Random Systems to be Evaluated

For each type of functional unit, 200 systems were randomly generated: 100 systems with 50 unit processes, and 100 systems with 100 unit processes. Each system was generated by starting at the functional unit and working upstream systematically adding unit processes to the system. To make each system as realistic as possible the following rules were used:

- The number of inputs to any unit process is from 1 to 6 with a triangular discrete probability distribution function, which gives 3 or 4 inputs the highest probability, and 1 or 6 inputs the lowest probability.
- The mass ratio of inputs to outputs for any unit process is from 1 to 5, meaning an optimal unit process could have 100% efficiency in mass transfer, whereas the worst unit process is one which requires 5 times the mass input to generate an output. The mass ratio is assumed to be uniformly distributed between 1 and 5.
- For each unit process, mass is conserved by assuming the combined total of input materials becomes either output products or environmental outputs (e.g. Environmental Outputs = Total Mass of Inputs – Total Mass of Products). These environmental outputs are assumed to be common combustion related emissions.

- The energy efficiency of a unit process is assumed to be uniformly distributed between 5% and 99% meaning in the best case a unit process will transfer 99% of its input energy to the product (the difference is lost to the environment).
- The energy per kilogram of any input or output is bounded between 0 and 50 MJ/kg. In other words, no material in the system can have a heating value above 50 MJ/kg.
- The market value of flows in each system is defined by a random rate of return for each unit process. The rate of return is assumed to be uniformly distributed between 0 and 20%. As a result, the Total Value of Inputs to a Unit Process = Total Value of the Product / (1 + Rate of Return).
- Co-products of a unit process are not generated for the random unit processes because it is assumed upstream inputs and environmental outputs have been allocated to each product. The resulting random system represents the allocation of inputs and environmental outputs to the primary product.

Evaluation of Random Systems

Each of the 800 random systems was evaluated at different Z_{RMEE} cut-off ratios in order to find a relationship between Z_{RMEE} and the fraction of the known total environmental output for any system. The total environmental output of each system was evaluated using a range of Z_{RMEE} cut-off ratios: $Z_{RMEE} = 0, 0.05, 0.10, 0.15, 2.0$. Each random system reacts differently with respect to how much of the known total environmental output is reported at different Z_{RMEE} values. Figure 3.6 provides an example of three independent random realizations of Type II systems and their relationship between the fraction of environmental output and the Z_{RMEE} cut-off.

The "true" total of environmental output for each system is found in the case where $Z_{RMEE} = 0$, hence in Figure 3.6 all three systems start with 100 percent of the environmental outputs at $Z_{RMEE} = 0$. As Figure 3.6 shows, different random systems of the same system type are affected differently by varying Z_{RMEE} ratios. The measured

output of some systems drops rapidly at low Z_{RMEE} , while others measure over 90% of the total environmental output even at $Z_{RMEE} = 2.0$. The objective here is to derive a trend between Z_{RMEE} and the fraction of total environmental output measured, by using large sets of random systems.

Each of the eight sets (50 and 100 unit process systems for each of the four system types) of 100 random systems were evaluated at Z_{RMEE} values ranging from 0 to 2 at increments of 0.05. Using these results a statistical evaluation was completed to determine if there is a significant difference between the eight sets of systems.



Figure 3.6: An example of 3 Type II Systems and the Relationship Between Z_{RMEE} Cut-Off Ratio and Fraction of the True Total Environmental Output



Figure 3.7: Comparison of the mean relationship between Z_{RMEE} and the fraction of total environmental output for each set of 100 random systems.

Comparison of each set of Random Systems

Figure 3.7 shows a plot of the average result for each of the eight sets of systems. To test the significance of the number of unit processes in a system, the mean of systems with 50 unit processes was compared to the mean of systems with 100 unit processes using T-statistic hypothesis testing.

The statistical test applied to the mean of each Z_{RMEE} value for each system type is shown in Equation 3.1. The Null Hypothesis (Ho) is defined as $U_{50} = U_{100}$ (the mean percent of total environmental output of a system with 50 unit processes is the same as the mean of a system with 100 unit processes for any given Z_{RMEE}). The Alternative Hypothesis (Ha) is $U_{50} \neq U_{100}$. The null hypothesis rejection region is defined as $T < -t_{\alpha/2}$ and $T > t_{\alpha/2}$, with significance level α . This is a two tailed statistical test with unknown variances and does not require equal variances between the populations [4]. Since 100 samples is relatively large, the normal distribution is assumed in the test by the law of propagation of errors [4]. Although the T statistic is designed for normal distributions it can be applied to nonnormal distributions as long as both samples are large enough for the central limit theorem to be invoked [5].

$$T = \frac{U_{50} - U_{100}}{\sqrt{\frac{S_{50}^2}{n_{50}} + \frac{S_{100}^2}{n_{100}}}}$$
(3.1)

U = Sample mean S = Sample standard deviation n = Sample size

The results of the statistical test at significance level α =0.05, show no evidence to reject the null-hypothesis. This means it is reasonable to assume the relationship between Z_{RMEE} and the percent of the true environmental output of a system is independent of the number of unit processes in the system. As a result, the sets of random systems with 50 and 100 unit processes were combined for each system type (Type I, II, III, and IV). Next, a comparison between each of the four types of systems was completed to determine if all 800 random systems could be considered together. Figure 3.8 provides an indication that the mean and 95% confidence intervals for each type of system are fairly closely grouped. To test this, the mean values of the four different types of systems were also compared using the statistical procedure in equation 3.1. The objective was to evaluate whether there is a significant difference between types of systems (each type defined by the mass, energy and market value of the functional unit). The statistical test again showed no evidence to reject the null hypothesis that the mean values of each of the four system types (I, II, III, IV) are equal. As a result, it is a reasonable assumption to combine the 800 random realizations of four different types of systems in order to calculate a mean and 95% confidence interval for the relationship between Z_{RMEE} and the fraction of total environmental output.



Figure 3.8: Comparison of the Mean and 95% Confidence Intervals for each of the four types of systems.

3.3.2 Results - The Relationship Between Z_{RMEE} and Fraction of Total Environmental Output

The mean and 95% confidence interval for the fraction of total environmental output reported at different Z_{RMEE} values is shown in Figure 3.9. This fraction of the total environmental output is defined as Y_{ZMean} with 95% confidence interval defined between Y_{ZHigh} (high value) and Y_{ZLow} (low value). Table 3.6 provides the same results with additional information including the standard deviation and mode at each Z_{RMEE} value.

Beyond $Z_{RMEE} = 0.5$, the lower 95% confidence interval for the fraction of environmental output measured drops below 50%. Based on the author's experience, it is not recommended to use Z_{RMEE} values greater than 0.25 because too much uncertainty is introduced to the analysis. The Z_{RMEE} values of most interest are from 0.05 through to 0.25 where more than 90% of the total environmental outputs are likely to be within the system boundary, and the lower bound of the 95% confidence interval remains above 70%.



Figure 3.9: Mean and 95% Confidence Interval for the Percent of Total Environmental Output (Y_{zMean}) reported at different Z_{RMEE} values.

Environmental Output for Different Z _{RMEE} values.							
	Percentage of True Total Environmental Output			Mode	Standard Deviation		
Cut-Off	Mean	High	Low	MRMEE	SRMEE		
Ratio	(Y _{zMean})	(Y _{zHigh})	(Y_{zlow})				
(Z _{RMEE})							
0	100.00	100.00	100.00	100	0		
0.05	99.38	99.97	96.67	99.90	0.93		
0.10	98.37	99.96	91.40	99.51	2.52		
0.15	97.29	99.93	85.33	99.45	3.86		
0.20	96.16	99.90	80.50	99.30	5.32		
0.25	94.74	99.85	74.60	98.78	7.05		
0.30	93.40	99.81	68.50	97.42	8.66		
0.35	91.74	99.76	62.00	97.33	10.40		
0.40	90.16	99.70	52.00	97.12	11.89		
0.45	88.58	99.63	44.67	96.13	13.40		
0.50	87.09	99.57	42.67	95.52	14.62		

Table 3.6:Mean and 95% Confidence Interval of the Fraction of Total
Environmental Output for Different ZRMEE values.

3.4 Application of the Results

The results presented in Figure 3.9 and Table 3.6 show a relationship between Z_{RMEE} and the ratio of the true total environmental outputs (Y_{ZMean}). This relationship can be used to estimate the uncertainty in results due to system boundary selection for real LCA analysis where the true environmental output is not known. Development of the relationship between Z_{RMEE} and Y_{ZMean} has been made with common combustion related air emissions. The RMEE method is well suited for these emissions because there is a strong corelation between the three RMEE criteria (mass, energy and economic value) and combustion emissions [1]. For LCA studies wishing to investigate toxicity issues, RMEE is not recommended.

Define X_{zj} as the mean total value of a given environmental pollutant (e.g. greenhouse gases) calculated for a given system (j) with system boundaries defined by Z_{RMEE} . The value X_{Zj} is the mean value of an environmental output calculated through a life-cycle inventory and will have a standard deviation and uncertainty due to data quality. Define the 95% confidence interval for X_{Zj} as \mathbf{r}_{data} (\mathbf{r}_{data} represents the propagation of error throughout the system due to uncertainty in the data of individual unit processes and is best calculated using Monte Carlo Analysis (MCA) [2]). Then, using the Y_{zMean} value for the given Z_{RMEE} in Table 3.6, and equation 3.2, it is possible to calculate $X_{zj}^{*}(X_{zj} \text{ primed})$ as an approximation of the true total environmental output. X_{zj}^{*} represents an estimation of the true environmental output for system j by taking into account the unit processes outside the system boundary. This is an approximation based on observation from the 800 random systems modeled to derive the relationship between Z_{RMEE} and uncertainty in system boundary. This equation is based on the relationship between Z_{RMEE} and the fraction of total environmental output (Figure 3.9, Table 3.6).

$$X'_{zj} = \frac{X_{zj}}{Y_{zMean} / 100}$$
(3.2)

X'zj = Approximation of the true mean of an environmental pollutant.
 X_{Zj} = Calculated environmental pollutant of system j with system boundary defined by Z_{RMEE}.
 Y_{ZMean} = The mean percent of the true environmental pollutant at Z_{RMEE}.

In order to calculate the total uncertainty associated with the results of an LCI, the uncertainty due to system boundary selection must be combined with the uncertainty due to data in the analysis (r_{data}). Because the distribution of Y_{ZMean} is non-normal, normal distribution statistics can not be used for combining the uncertainty from data, with the uncertainty introduced due to system boundary selection. Figure 3.10 illustrates the type of skewed distribution Y_{ZMean} follows. This distribution is typical for all Z_{RMEE} values.



Figure 3.10: Illustration of the non-normal distribution of YZMean.



Figure 3.11: Illustration of the truncated-normal distribution used to approximate the numerical probability distribution function for Y_{ZMean}.

To combine the uncertainty from data (r_{data}) with uncertainty introduced due to the distribution of Y_{zMean} , Monte Carlo Analysis has been used to calculate the mean and uncertainty of X'_{Zj}. Using equation 3.2, 1000 random variables from the distributions of X_{Zj} and Y_{zMean} are selected to generate a distribution for X'_{Zj}. From the distribution of X'_{Zj} the mean and 95% confidence interval is calculated to provide a best approximation of the total outputs of an environmental pollutant in an LCA.

In order to complete the Monte Carlo Analysis on equation 3.2, a probability distribution function must be selected for Y_{zMean} . For this research, two probability distribution functions were tested and compared:

- the distribution generated numerically from the 800 random systems (illustrated by Figure 3.10), and
- a normal distribution centered on the mean and truncated at Y_{zMean} equal to 100 with values greater than 100 placed at the upper boundary (Y_{zMean} = 100), as illustrated in Figure 3.11.

The example below shows three things:

- 1) as Z_{RMEE} is reduced the total uncertainty is reduced,
- the truncated-normal distribution provides a conservative estimate of the uncertainty when compared to the numerically generated probability distribution function, and
- 3) how to complete a comparison between two random systems System B and System C, using the RMEE method. It is also shown how to estimate the probability the mean environmental outputs of one system is less than a competing system.

3.4.1 An Example of Applying the System Boundary Factor (Y_{zMeen}) and System Boundary Uncertainty Estimated by RMEE

For this example, two random systems were generated consisting of 100 unit processes. Both systems produce the same functional unit with a heating value (25 MJ/kg) and market value (\$1/kg) (Type I). These systems have been called "System B" and "System C". For illustrative purposes, only greenhouse gas emissions are evaluated in this example.

The Relationship Between Overall Uncertainty and ZRMEE

Figures 3.12 and 3.13 illustrate the relationship between the Z_{RMEE} value and the change in mean greenhouse gas emissions and uncertainty for System B and System C. As the Z_{RMEE} value increases the analysis becomes less detailed and more unit processes or sources of pollutants are left outside the system boundary. The RMEE method increases the uncertainty in results as Z_{RMEE} increases to reflect the change in system boundary.



Figure 3.12: The relationship between the Z_{RMEE} value and mean with 95% confidence interval for System B. At $Z_{RMEE} = 0$, the only source of uncertainty is from uncertainty in the data.



Figure 3.13: The relationship between the Z_{RMEE} value and mean with 95% confidence interval for System C. At $Z_{RMEE} = 0$, the only source of uncertainty is from uncertainty in the data.

Comparison of Applying the Numerically Generated Probability Distribution Function and the Truncated-Normal Distribution

For widespread application of the RMEE method, the tool must be practical. As a result, it is desirable to utilize a probability distribution function, which approximates the numerically generated distribution from this research. It is generally accepted that the normal distribution is one of the more readily applied distributions in engineering and science. To approximate the skewed distribution of Y_{ZMean} , this analysis uses a normal distribution truncated at Y_{ZMean} =100 where any values greater than 100 are placed at the 100 boundary. Figure 3.11 illustrates the distribution being used compared to the shape of the numerically generated distribution illustrated in Figure 3.10.

Figure 3.14a illustrates the difference between using the numerically generated probability distribution function for Y_{ZMean} in equation 3.2 and using a truncated-normal distribution. The comparison tends to indicate that using the truncated-normal distribution results in a more conservative approximation of the 95% confidence interval. Figure 3.14a also shows that as Z_{RMEE} increases, the overestimation of the truncated-normal increases. At $Z_{RMEE} = 0.50$, use of the truncated-normal distribution. However, at Z_{RMEE} values between 0.05 and 0.25 (these are the values of Z_{RMEE} of most interest – see section 3.3.2 above), use of the truncated-normal distribution provides a conservative representation of the numerically generated distribution and the truncated normal distribution of uncertainty tend to follow a semi-log process as Z_{RMEE} increases. This is shown in Figure 3.14b.

Because the truncated-normal distribution results in a conservative approximation of the 95% confidence interval and is relatively easy to generate, it is recommended that this distribution be applied for the RMEE method. This will help ensure the RMEE method is practical for LCA application. As a result, the remainder of this research applies the truncated-normal distribution for the distribution of Y_{ZMean} when applying Monte Carlo Analysis to equation 3.2.

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Distribution Function for Different Zrmee Values

Figure 3.14a: Comparison of applying the Truncated-Normal (Trunc Norm) distribution function to the numerically generated distribution function (Num) for various Z_{RMEE} values. The values shown represent the mean and 95% confidence interval for System B.



Distribution Function for Different Zrmee Values

Figure 3.14b: Log-Normal plot comparing the Truncated-Normal (Trunc Norm) distribution function to the numerically generated distribution function (Num) for various Z_{RMEE} values. The values shown represent the mean and 95% confidence interval for System B.

Applying the RMEE Method to Compare Two Systems

Consider the LCA practitioner who decides to begin with a Z_{RMEE} value of 0.25. This means any flow in the system with a mass, energy and market value which is less than one-quarter of the functional unit's mass, energy and market value will be left outside the system boundary. The calculated results at $Z_{RMEE} = 0.25$ for System B and System C are shown in Figure 3.15 with mean (X_{25j}) and uncertainty (r_{data}). These results are based only on the calculation of greenhouse gases from available data. No adjustment has been made to the results for system boundary selection. The results show System C to result in less greenhouse gases with partial overlap of uncertainties.



Figure 3.15: Mean and 95% Confidence Interval of System B and System C at $Z_{RMEE} = 0.25$ before adjusting for system boundary selection.

The next step is to adjust the initial calculated mean and uncertainty to take into account system boundary selection. This is accomplished by using Monte Carlo Analysis to combine the distribution of Y_{25Mean} and the distribution of X_{25j} for each system. The "RMEE Adjusted" comparison between System B and C after accounting for the system boundary are shown in Figure 3.16. This result has been generated using the truncated-normal probability distribution function for Y_{25Mean} .


Figure 3.16: RMEE Adjusted Comparison of the mean and 95% confidence interval of greenhouse gases from System B and System C at Z_{RMEE}=0.25 using the truncated-normal probability distribution function.

The results at $Z_{RMEE} = 0.25$, illustrated in Figure 3.16, show a significant overlap of uncertainties. Although a decision maker may typically visually assess the degree of overlap in uncertainty and a make a decision, it is helpful to quantify the probability one option results in less environmental output than another.

One can quantify the probability that System C is less than System B. If the results from each system are normally distributed with the same standard deviations, one can use the normal distribution tables to quantify the probability the mean emissions from System C are less than the mean emissions from System B. Area (I) in Figure 3.17 represents this probability.

However, because the distribution of X_{z_j} ' is not normal, Area (I) is best approximated by placing the results of the Monte Carlo Analysis into histograms and numerically calculating Area (I). Area (I) estimates the probability of the mean of System C being less than the mean of System B and is calculated using Equations 3.3 and 3.4.

 $Area(I) = \sum_{i=1}^{N} (F_i^{C} - F_i^{B})$ $F_i^{C} = Frequency of the Environmental Output of System C in Bin i$ $F_i^{B} = Frequency of the Environmental Output of System B in Bin i$ N = Number of Bins in the histogram.(3.3)

$$P(P_{ZC} < P_{ZB}) = \frac{\sum_{i=1}^{N} (F_i^{C} - F_i^{B})}{\sum_{i=1}^{N} (F_i^{C})} = \text{Probability } P_{ZC} \text{ is less than } P_{ZB}$$
(3.4)

 P_{ZC} , P_{ZB} = Mean Environmental Pollutant Output of System C and B.



Figure 3.17: Area (I) Represents the Probability the Mean of System C (X_{ZC}') is Less than the Mean of System B (X_{ZB}').

Applying this technique to Systems C and B at $Z_{RMEE} = 0.25$ results in a 57.5% probability of the mean of System C being less than the mean greenhouse gas emissions of System B. For decision making, one may wish to expand the system boundary in order to further reduce the uncertainty in the decision. This is completed by reducing Z_{RMEE} and re-evaluating the system.

Figure 3.18 presents the comparison at $Z_{RMEE} = 0.10$. At $Z_{RMEE} = 0.10$, the system is expanded to the point at which the uncertainty associated with system boundary selection

is significantly reduced. It is found to be 64.7% probable that the mean of System C will be less than the mean greenhouse gas emissions of System B. At this point, the decision maker has greater confidence in making the decision, but may still wish to further expand the system boundary.



Figure 3.18: RMEE Adjusted Comparison of the mean and 95% confidence interval of greenhouse gases from System B and System C at Z_{RMEE}=0.10 using the truncated-normal probability distribution function.

If the boundary is further expanded by using $Z_{RMEE} = 0.05$, the uncertainty is further reduced as shown in Figure 3.19. At this level of detail, the results show it is 76.2% probable that the mean of System C will be less than the mean of System B. To further reduce uncertainty requires reducing the uncertainty in data.



Figure 3.19: RMEE Adjusted Comparison of the mean and 95% confidence interval of greenhouse gases from System B and System C at Z_{RMEE}=0.05 using the truncated-normal probability distribution function.

3.5 The RMEE Adjustment for a Significantly Different Type of System

The results presented here were developed by analyzing a large number of random systems which followed specific rules, defined in the section above entitled "Random System Generation". These rules require each unit process to conserve mass. This would be true for a typical manufacturing or material handling unit process. However, in the practice of LCA, some unit processes exist which do not conserve mass, due to the method of inventory assessment. For example, an LCA studying biomass production systems, such as corn production, would typically not have a mass balance because carbon from the soil and air, rain water, and many other naturally occurring nutrients which produce the corn are not normally accounted for in the life-cycle inventory. As a result, unit processes exist which produce a high mass product with relatively minor levels of measured inputs such as diesel fuel, fertilizers, and pesticides.

To test the impact on the RMEE method of unit processes which do not balance mass, two hundred systems were generated using the same rules as above, except that the mass ratio of inputs to outputs for any unit process could range from 0.1 to 5. In other words, a unit process could produce more mass in products than the measured mass of inputs. The results for this scenario are shown in Figure 3.20 and Table 3.7, where it can be seen the average fraction of environmental outputs measured within the system boundary decreases more rapidly with the increase in Z_{RMEE} . The numbers presented in Table 3.6 for non-biomass systems, Y_{ZMean} crosses the 90% level at $Z_{RMEE} = 0.4$, while for the biomass systems presented in Table 3.7, Y_{ZMean} crosses the 90% point much earlier at $Z_{RMEE} = 0.2$.

In summary, the RMEE method provides a method of quantifying the uncertainty associated with system boundary selection. However, the results presented here show some influence of the nature of the system, particularly for systems which deviate greatly from the norm.



Figure 3.20: Mean and 95% Confidence Interval for the Fraction of Total Environmental Output (Y_{zMean}) reported at different Z_{RMEE} values for Biomass Type Systems.

Systems							
	Perce Env	Standard Deviation					
Cut-Off	Mean	High	Low	SRMEE			
Ratio	(Y _{zMean})	(Y _{zHigh})	(Y _{zLow})				
(Z _{RMEE})							
0	100.00	100.00	100.00	0.00			
0.05	98.01	99.95	89.00	3.06			
0.10	95.44	99.91	68.50	7.89			
0.15	92.66	99.86	53.00	12.21			
0.20	90.48	99.81	49.00	13.51			
0.25	87.05	99.71	28.00	17.62			
0.30	84.85	99.62	23.00	18.79			
0.35	82.69	99.38	22.50	19.78			
0.40	79.77	99.38	17.00	22.62			
0.45	78.18	99.29	11.00	23.96			
0.50	77.08	99.00	8.50	24.38			

Table 3.7:Mean and 95% Confidence Interval of the Fraction of Total
Environmental Output for Different Z_{RMEE} values for Biomass Type
Systems

3.6 Conclusions

- The RMEE method of system boundary selection allows for the quantification of system boundaries and the evaluation of the uncertainty due to system boundary selection which is introduced to the results of an LCA. RMEE has been specifically designed and tested for energy and product systems in which an evaluation is being made on common combustion air emissions.
- The RMEE method provides an adjustment factor (Y_{zMean}) which can be used to adjust the results of an LCA to account for unit processes excluded from the system boundary at a chosen Z_{RMEE}.
- The uncertainty introduced from system boundary selection is related to Z_{RMEE} and increases as Z_{RMEE} increases. The relationship is shown in Figure 3.9 and tabulated in Table 3.6.
- The probability distribution of Y_{zMean} is a skewed non-normal distribution.
- A truncated-normal distribution is considered to provide a fair representation of the numerically generated distribution (skewed non-normal) for Z_{RMEE} values less than or equal to 0.25.

- Monte Carlo Analysis is recommended as the most practical method to combine the uncertainty associated with Y_{zMean} and uncertainty due to data in X_{zj}.
- Calculating the probability the mean environmental outputs of one system is less than the mean of a competing system can be accomplished by comparing the histograms generated by the results of the Monte Carlo Analysis.
- The RMEE method provides consistent measures of system boundary related uncertainty for the most common classes of individual systems. However, production systems with significantly different characteristics (such as biomass production systems) provide a wider range of uncertainty. This result is shown in Figure 3.20 and tabulated in Table 3.7.

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Chapter 4

Assessing Error Propagation in Life-Cycle Assessment Systems

The second primary objective of this research is to investigate and develop tools which handle uncertainty in the data of life-cycle assessment (LCA) studies. Chapters 2 and 3 showed how the selection of the system boundary is one source of uncertainty due to methodology. Section 4.1 shows uncertainty can enter in the results of an LCA through data and through methodology. This chapter presents a method to calculate the overall uncertainty due to the propagation of uncertainty in individual unit processes.

Section 4.1 is a paper published by the Society of Automotive Engineers at the 1999 International Congress and Exposition. It discusses the sources of uncertainty in LCA and provides an overview of current methods of dealing with uncertainty in the LCA field. The paper demonstrates the application of Monte Carlo Analysis to evaluate uncertainty in the life-cycle inventory (LCI) stage of LCA. It also defines a method to identify the most significant unit process in a system with respect to their contribution to overall uncertainty. These two uncertainty tools are valuable in helping to streamline LCA decision making and to gain a better understanding of the uncertainty in the conclusion.

Sections 4.2 and 4.3 present further analysis which arose from discussion of the SAE paper in 4.1. Section 4.2 revisits the number of iterations required to complete Monte Carlo Analysis to ensure convergence occurs during modeling. The final section of this chapter, section 4.3, investigates the cases in which LCA modeling becomes a non-linear process.

4.1 – APPLICATION OF MONTE CARLO ANALYSIS TO LIFE CYCLE ASSESSMENT

[Published at SAE Congress 1999 – Paper Number 99ENV-20]

4.1.1 Introduction

Life cycle assessment (LCA) is a systematic decision making and design tool which evaluates the impact of a product or service by considering all stages from raw material acquisition through manufacture, use and disposal. Thus LCA analysis is commonly referred to as "cradle-to-grave" analysis. LCA has received global attention through the development of the ISO 14040 standards for LCA as a tool within an environmental management system [2]. A broad range of industries have applied LCA in decision making and design, including the automotive industry, utilities, oil and gas, product packaging, and others [4] [18].

Over the past 20 years of development, LCA methodologies have evolved and have been refined. However, in all LCA methods substantial amounts of input data are used to produce similarly substantial numbers of outputs at the "inventory assessment" stage of LCA [2]. Some degree of uncertainty about the actual values and about the applicability of those values to the problem at hand is inherent with any set of data used for decision making. The uncertainties in individual data points within the LCA are combined and propagated through the process to create an overall uncertainty in the results of an LCA. It is important for decision makers using LCA to understand the degree of uncertainty in results in order to make better-informed decisions.

The importance of properly assessing the uncertainty in LCA results has been expressed by a number of authors [1][2][4]. However, LCA techniques, as used at present, do not adequately address uncertainty in their data sets or LCI, methods of computation, computed results or conclusions. As described by *Besnainou and Coulon* in *Curran's* book on Life-Cycle Assessment [4]:

"in communicating to audiences aware of the complexity and uncertainty underlying the final results – fast becoming the bulk of the decision-making and policy-making audience – LCA currently can provide no information about ranges or levels of confidence in the results." [4]

This paper can not solve all of the concerns and issues around uncertainty in LCA. However, its purposes are to identify the sources of uncertainty in LCA, to present current practices of uncertainty analysis, to provide a robust method of evaluating the propagation of error through a life cycle assessment, and to provide a method to identify the relative significance of the uncertainty associated with each unit process in a system.

4.1.2 Sources of Uncertainty in LCA

Uncertainty in the results of an LCA can be broken into two distinct categories: 1. uncertainty in system input and output data, and 2. uncertainty generated from procedures for calculations.

Uncertainty in System Data

Data quality has always been an issue for LCA practitioners. Data quality directly affects the life-cycle inventory (LCI) stage of LCA. This is illustrated by the number of publications on the topic [5][6][7][8][16][17]. "Quality" here is defined as the accuracy of the data for the purpose of the LCA. The literature provides numerous examples and methods for rating the data quality of individual data points through various "Data Quality Indicators" (DQIs). The qualitative DQI systems provide a means to monitor the relative quality of data being used in an LCA. However, these methods of assessing data quality are not sufficiently quantitative to help the decision makers who ultimately use the results of an LCA answer. Their question is, (or should be): "What band of uncertainty can I expect around the result of this LCA?"

The literature has identified and described the potential sources of uncertainty in data through its development of DQIs. Table 4.1 summarizes the DQIs, which identify potential sources of uncertainty.

DQI / Data Quality Requirement	Description			
time-related coverage	the age of data compared to the study period	[1]		
geographical coverage	the geographical area from which data is collected	[1]		
technology coverage	the technology mix from which the data is collected compared to the technology utilized by the systems being assessed	[1]		
precision	the measure of the variability of the data values	[1][16]		
completeness	the percentage of locations reporting primary data from the potential number in existence	[1][16]		
representativeness	Qualitative assessment of the degree to which the data set reflects the true population of interest (i.e. geographical coverage, time period and technology coverage)	[1] [16]		
applicability/suitability/ compatibility Relevance of the data set within a study to the purpose of that study. Requires analysis of data sources, data types, age of data, and of the technology match between data source and study target.		[16]		
bias	systematic or nonrandom deviation or error that makes data values consistently higher or lower than they should be.	[16]		
stability	Measure of consistency and reproducibility of data over time.	[16]		

 Table 4.1:
 Data Quality Indicators Identifying Potential Sources of Uncertainty in LCA Data

The challenge for the field of LCA has been to develop a repeatable method which moves beyond a simple set of data quality indicators and provides a quantified uncertainty value for the LCI stage. At the current time, the LCI is completed with no quantitative measure for the range of uncertainty in their results. As a result, current best practice is to utilize "expert judgement" on the uncertainty for any particular data point. Because of the large number of data points in an LCI, and because the propagation of uncertainty throughout the system can significantly affect the overall accuracy of a study [4], there is a critical need to develop a more rigorous method of assessing uncertainty in the LCI.

Methodological Sources of Uncertainty

Uncertainty in the overall results of an LCA can enter through the LCA method applied and through the method of calculating the propagation of error in a life cycle system, regardless of the uncertainty level in the data itself. ISO 14041 recognizes this methodological source of uncertainty by defining a descriptor for data quality called: "consistency: qualitative assessment of how uniformly the study methodology is applied to the various components of the analysis;" [1][16].

One of the sources of methodological uncertainty is the means by which the system boundary is selected for a life cycle system [5]. In theory, the complete "cradle-to-grave" life cycle of any given product or service is linked indirectly to the entire global economy. To make a practical analysis, every LCA needs to define a limited system boundary that encompasses the most relevant unit processes and quantify the impact of those processes within that boundary. The material and service flows and the environmental impacts of those unit processes outside of the system boundary are not accounted for in the final results of an LCA (refer to Figure 4.1). The unmeasured value of the excluded impacts introduces an uncertainty to the results and conclusions of the LCA based on any reasonable system boundary. This becomes more problematic when two or more products or services are compared since the method of system boundary selection for the different systems may not set comparable boundaries. The result of not consistently selecting system boundaries is the introduction of different degrees of uncertainty to the results of different systems [10][11]. For example, consider a LCA comparing an electric vehicle to an internal combustion gasoline vehicle. For each option a system boundary will be selected, introducing uncertainty to the results due to the impacts of unit processes falling outside the system boundary. Should the electric car system include metal mining, metal smelting and metal recycling for battery materials? Should the gasoline car system extend as far as the original resource exploration to find petroleum reservoirs? How significant is the impact of each unit process which falls outside the system actually analyzed and could this affect the LCA comparison between two products?

The LCA practitioner has a practical requirement to ensure that a similar degree of uncertainty is introduced for each system analyzed. Furthermore, the value of this uncertainty must be estimated in a reliable manner. A number of methods have been suggested for selecting system boundaries [10], none of which address the issue of uncertainty. RAYNOLDS *et al* [9][10] have developed a method of system boundary selection which ensures comparable system boundaries are selected for different options in an LCA. Work presented by RAYNOLDS *et al* [11] shows the relationship between system boundary selection and uncertainty.

A second source of methodological uncertainty is through the models used to translate inventory results to aggregate impacts such as environmental indicators or stressor categories. For example, the total emissions of carbon dioxide, CFC's, methane, water vapour and nitrous oxide are commonly aggregated to give a greenhouse gas emission value. The weighting factors used to convert various emissions into a carbon dioxide equivalent introduce an unknown amount of uncertainty. Is methane actually 21 times as effective as carbon dioxide at causing global warming [Intergovernmental Panel on Climate Change (ICPP)]? Or is the factor 32? Such aggregation ratios can have a significant impact on LCA studies comparing products or processes which shift the balance between different emissions. A similar question arises with impacts such as economic activity or emissions produced at different locations or different times. Should such impacts be aggregated directly? Or should there be some weighting factor for spreading or deferring the effects of a process? The methods of LCA impact assessment are currently in development and practical science must address the issue of uncertainty in its models.

A final example of uncertainty from LCA methodology is the calculation method applied to actually measure the overall uncertainty in an LCA. In other words, the method of calculating the propagation of error throughout a life cycle system is a source of uncertainty itself. At the present time, different methods are being used to calculate the error propagation in LCA. This leads to uncertainty in the reported uncertainty! This paper reviews current methods and describes in detail the application of Monte Carlo analysis for calculating uncertainty.



Figure 4.1: System Boundary Selection and Uncertainty

4.1.3 Current Methods of Dealing with Uncertainty in LCA

The most common method of dealing with uncertainty in the results of an LCA is to simply assume that differences in results between options must be greater than 10 or 20 percent to represent a significant difference [4]. Due to the number of data points in a typical LCA study and the propagation of error throughout the system it is easily foreseeable that uncertainty could exceed 20 percent. As LCA becomes a more widely used tool for decision making it will become more important to accurately quantify uncertainty. ISO 14041 suggests calculating uncertainty and defines uncertainty analysis as:

"a systematic procedure to ascertain and quantify the uncertainty introduced into the results of a life cycle inventory analysis due to the cumulative effects of input uncertainty and data variability; NOTE – either ranges or probability distributions are used to determine the uncertainty in the results." [1]

In cases where uncertainty of individual data points has been estimated or calculated, various methods of calculating the overall uncertainty due to error propagation have been applied. As a first estimate, work completed by *Raynolds et al* [12] calculated the overall uncertainty (95% confidence interval) in system results using Equation 4.1.

The cumulative uncertainty or error (r_{Total}) is calculated by the following weighted averaage equation:

$$r_{Total} = \left(\sum_{i=1}^{n} \frac{x_i}{X} (r_i)^2\right)^{1/2}$$
(4.1)

with

n = number of unit processes

 x_i = mean value for unit process i

- X = system total of means i.e. summation x_i
- $r_i = error$ in mean of unit process i

This commonly used error summing method is based on an assumption that errors in all unit processes are small and independent of one another. It is also only appropriate for symmetric distributions, which poses a significant limitation. As such, it does not properly account for error propagation generated by the connection and interaction of material and energy flows between unit processes. Given this, Equation 4.1 is only an approximation of the uncertainty level in LCA study results.

A similar approach has been applied in calculating the uncertainty in greenhouse gas emissions for Canada's 1990 emissions [15] where overall uncertainty was estimated by:

Total Uncertainty = $\sqrt{(UA^2 + UB^2 + ...)}$

where UA, UB, etc. is the uncertainty in data points A, B, As mentioned, this method is only appropriate for combining uncertainties where the sources are completely independent. In addition, MCCANN [15] noted that this method is not statistically correct for cases with large uncertainties and recommends the use of Monte Carlo analysis.

The use of Monte Carlo analysis for LCA has been researched and described by KENNEDY et al [7]. They translate a set of data quality indicators to a distribution function for each data point which is then utilized in a Monte Carlo analysis. Their Monte Carlo analysis iterated the evaluation 100 times using a beta function for the probability distribution [7]. This study was a valuable step towards providing LCA practitioners with a practical means of translating expert judgement on data quality to a quantified range of uncertainty. KENNEDY et al identified two areas which required further research [7]:

- 1. "The final impact of the cascading uncertainty associated with the aggregation of input data from multiple levels of LCA inventory modeling requires additional analysis.", and
- 2. "a method needs to be developed to analyze the LCA inventory model input data to identify those data elements that significantly contribute to the variance of the results."

This paper attempts to address these two areas.

4.1.4 Cascading Uncertainty - Revisiting Monte Carlo Analysis

Life cycle assessment is a simulation tool – models of real systems are used to predict and compare the overall environmental performance of systems which produce similar products or services. Simulation is one of the most powerful tools for designing and assessing complex systems [13][14]. In comparison to analytical methods, simulation allows the decision-maker to better see and "play" with systems, leading to a deeper understanding of the systems and their impacts [14]. As a result, simulation is the most widely used quantitative technique for problem solving [14]. The simulation generated by an LCA can be used to run a Monte Carlo analysis and estimate the overall uncertainty in the LCA results when reasonable but randomly varying values are used for system inputs.

The name Monte Carlo originates from the city on the Mediterranean with its famous casino because Monte Carlo analysis uses random numbers (such as numbers generated in a casino) to study a problem [3]. The advantage of Monte Carlo methods over analytical methods is that very complicated systems can be analyzed using relatively simple calculations and without requiring a deep understanding of statistical analysis theory [3]. For LCA practitioners and decision makers using the results of an LCA, Monte Carlo analysis provides the most practical and accurate method of calculating the overall uncertainty in an LCA due to error propagation.

Research of RAYNOLDS *et al* [10][11] on selection of system boundaries and on assessing the relative environmental impact for alternative automotive fuels [9] utilizes Monte Carlo analysis to assess the uncertainty in overall results. For a typical unit process, three sets of ratios are defined to have a degree of uncertainty associated with them (refer to Figure 4.2):

- 1. the set of ratios I_{ij} / P_i between the various material and service inputs (I_{ij}) to a unit process and the primary product or service (P_i) of the unit process,
- 2. the set of ratios x_{ij} / P_i between the various environmental outputs (x_{ij}) of a unit process and the primary product of the unit process (P_i), and

 the set of ratios C_{ij} / P_i between the various co-products (C_{ij}) of unit process and the primary output (P_i), of a unit process.

It is these three sets of ratios $(I_{ij} / P_i, x_{ij} / P_i, and C_{ij} / P_i)$ which must be stochastically generated from a probability distribution function for the Monte Carlo analysis. The probability distribution chosen for these studies is the Gaussian or normal distribution. The reason for assuming a normal distribution is one of practicality. In most cases adequate samples of data are not available to generate a specific probability distribution function so some pre-defined mathematical function must be used. At this point, there is also insufficient information to justify complex distributions. Most data sources provide only a single value with no confidence range. Some sources describe the range of uncertainty in terms of a plus and minus range with a particular confidence interval. Given the level of uncertainty, the normal distribution is the most practical choice since it can be specified using only a mean value and a single measure of variance. Assuming a normal distribution simplifies the calculation of uncertainty but also becomes a source of uncertainty itself [15]. An alternative is to apply the methodology developed by KENNEDY et al [7] to translate a set of DQI's to the beta distribution. However, due to the lack of data available to generate probability density functions for each of the numerous (often 1000's) data points in a typical LCA, a Gaussian normal distribution is assumed.

To use Monte Carlo analysis for estimating the overall uncertainty of a life cycle system, the model must be run through a sufficient number of iterations to converge on a mean value. In the work completed by KENNEDY *et al* [7], the stochastic model was run for 100 iterations. How is the required number of iterations determined? For this study, the Monte Carlo analysis was applied to a fully defined model system called "System A", the details of which are shown in Figure 4.5. By fully defining a system, its actual output and the effect of data uncertainties on that output can be calculated analytically. The capability of the Monte Carlo analysis to predict that output and uncertainty can then be used as a test of the Monte Carlo technique. By applying the Monte Carlo analysis technique to "System A", it was found at least 1000 iterations were required for both the

mean and variance values to converge. This is illustrated in Figures 4.3 and 4.4 which were produced by applying a Monte Carlo analysis to the fully defined LCA system, "System A". To ensure adequate convergence with real systems, 2000 iterations were used for the Monte Carlo analysis technique applied in this study.

Table 4.2. Input and Output values for the runy behave system, system re-							
Unit Process (i)	Product	is (P _i)	Inputs (I _{ik})		Environmental Outputs (x _{il})		
	Flow	Amount	Flow	Amount	95% Confidence	Amount	+/- %
	Туре		Туре		(+/- %)		Uncertain
UP1	P ₁	50	P ₂	22	15	18	12
			P3	8	7		
UP2	P ₂	12	P4	5	5	35	10
			Ps	18	11		
UP3	P3	120	P ₆	210	20	51	15
UP4	P4	25				40	8
UP5	P5	40				10	18
UP6	P ₆	70				16	5

Table 4.2: Input and Output Values for the Fully Defined System, "System A"

Notes: $I_{ik} = An$ input to unit process "i" of flow type "k", i.e. P_k $x_{i1} = Environmental output from unit process "i" of type "1" e.g. CO₂ emissions.$

To test the accuracy of the Monte Carlo analysis, the uncertainty for System A was also calculated analytically using the general formula shown in equation 4.2:

For a function f(x,I),

$$(df)^{2} = \left(\frac{\partial f}{\partial x}\right)^{2} dx^{2} + \left(\frac{\partial f}{\partial I}\right)^{2} dI^{2}$$
(4.2)

where df is the uncertainty of f(E,I).

As an example consider the function of the total emissions for System A (equation 4.3). Using the input and output values for System A listed in Table 4.2, the mean value of the system environmental output (X) is calculated as 223.37 units. Table 4.3 summarizes the environmental outputs from "System A". Applying the general Equation 4.2 to Equation 4.3, with the uncertainty of the value of the functional unit (P_{Fn}) and all unit process products (P_i) set to zero, df is calculated analytically to equal 29.82. Thus, for "System A", the total environmental outputs calculated analytically is 223.37 +/- 13.35 %.

Total Emissions = $X = f(P_{Fn}, P_1, P_2, P_3, P_4, P_5, P_6, I_{12}, I_{24}, I_{25}, I_{13}, I_{36}, x_{11}, x_{21}, x_{31}, x_{41}, x_{51}, x_{61})$

$$X = f = \frac{P_{F_n}}{P_1} \left[x_{11} + \frac{I_{12}}{P_2} \left(x_{21} + \frac{I_{24}}{P_4} x_{41} + \frac{I_{25}}{P_5} x_{51} \right) + \frac{I_{13}}{P_3} \left(x_{31} + \frac{I_{36}}{P_6} x_{61} \right) \right]$$

Unit Process	Environmental Output	Percent of Total Emissions (X)
UP1	36.00	16.1%
UP2	128.33	57.6%
UP3	29.33	13.1%
UP4	16.5	7.4%
ŪP5	6.8	3.0%
UP6	6.4	2.9%
Total:	223.37	99.9%

Table 4.3: Environmental Outputs of "System A"

Monte Carlo analysis applied to "System A" with 2000 iterations gave the result:

Mean = 222.87 Uncertainty = +/- 13.50%.

The difference between the expected mean (223.27) and the value calculated by the Monte Carlo analysis (222.87) was 0.18%. The difference in the calculation of uncertainty was 0.15%.

In short, a Monte Carlo analysis using 2000 iterations provided a robust method of evaluating the effect of error propagation throughout and generating an estimate for the overall uncertainty in LCA results. As further research provides efficient methods of generating appropriate distribution functions for unit process input and environmental output data, the Monte Carlo method described above will be open to incorporate these advancements.

(4.3)



Nomenclature: The subscript nomenclature used in this paper is "i" = unit process number, "j" = input or output number for unit process i.

Figure 4.2: Inputs and Outputs of a Typical Unit Process



Figure 4.3: Mean Value of "System A" Emissions Converges With Increasing Number of Iterations



Figure 4.4: Uncertainty of "System A" Emissions Converges With Increasing Number of Iterations



Notes: P_k = flow of a product or service e.g. steel, power, etc.

 x_{ij} = environmental output of type "j" from unit process "i".

Figure 4.5: Process Flow Diagram for the Fully Defined LCA System, "System A"

4.1.5 Contribution to Overall Uncertainty- Uncertainty Reduction Analysis

As KENNEDY et al [7] pointed out, a method is required to determine which data points in a life cycle system are the most significant contributors to the overall uncertainty in results. This provides a valuable tool because it directs the practitioner to the data points requiring the highest quality of data (or at least the most improvement in data quality). This allows the practitioner to focus on reducing the uncertainty of the most relevant data points in order to reduce the overall uncertainty in results, leading to a better ability to discriminate between alternative systems. The method described here identifies the relative contribution of each unit process to the overall uncertainty in results of a life cycle system.

By running a complete Monte Carlo analysis for a system n times, where n is equal to the number of unit processes in the system, and for each run setting the uncertainty of a different unit process equal to zero, it is possible to evaluate the contribution of each unit process to the overall uncertainty. For example, when the Monte Carlo analysis for System A is run 6 times, each time with a different unit process's uncertainty set to zero, it is possible to identify which unit processes have the largest impact on the uncertainty. Table 4.4 summarizes the change in uncertainty as the uncertainty of each unit process in System A is set to zero. This is analogous to answering the question: "How much will the uncertainty in my results be reduced if I can get rid of all the uncertainty in unit process X?".

Table 4.4:	The Change in "System A" Uncertainty With Uncertainty of Each
	Unit Process Set to Zero

Uncertainty
56%
10%
negligible
negligible
negligible
negligible

Note: The uncertainty of **both** the environmental outputs (x_{i1}) and material inputs (I_{ij}) are set to zero.

From Table 4.4 it is possible to identify UP1 as the most significant contributor to the overall uncertainty – the uncertainty in the total results of the environmental outputs from "System A" will be reduced to 5.97% (56% reduction from original uncertainty of 13.5%). As a result, the practitioner is directed to focus first on obtaining better information for UP1 rather than spending excessive time or resources on the other unit processes. It is interesting to note that although UP2 contributes over 57% of the environmental outputs (refer to Table 4.3), reducing the uncertainty associated with UP2 to zero only reduces the uncertainty in the results by 10%. This could be counterintuitive to the LCA practitioner who sees 57% of the environmental output from UP2 and decides to focus on improving the data quality of UP2. The reason UP1 has the greatest impact on the overall uncertainty is the uncertainty in its inputs (I₁₂, I₁₃) propagates back through the entire system. UP2 produces more environmental impact but its uncertainty affects only part of the system.

The above method of systematically setting the uncertainty of the inputs and environmental outputs of individual unit processes in a system, combined with Monte Carlo analysis, is a practical method of identifying where to focus time and resources for reducing overall system uncertainty.

4.1.6 Conclusions

Based on the work completed, the following conclusions are made:

- 1. Monte Carlo analysis is an appropriate method for calculating the overall uncertainty in a life cycle system due to the propagation of error.
- 2. The mean system impact and the uncertainty in system impact converge after about 1000 iterations for a simple system. Running a Monte Carlo analysis with at least 2000 iterations, (or running a convergence test with varying number of iterations), is recommended to ensure convergence.
- 3. Systematically removing the uncertainty for individual unit processes gives Monte Carlo analysis the capability to identify the contribution of individual unit processes to the uncertainty of overall system output. This directs the LCA practitioner to focus on improving unit process data quality at the most relevant points. This technique has been called "Uncertainty Reduction Analysis" by the author.
- 4. Further research is required to develop rules for translating a practical set of data quality indicators into probabilistic distribution functions for unit process variables.

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4.2 – Additional Analysis of Monte Carlo Analysis Convergence

The paper presented in Section 4.1 demonstrated that more than 2000 random iterations of the Monte Carlo Analysis are required to guarantee convergence of the mean and uncertainty (shown in Figure 4.3 and Figure 4.4 of Chapter 4.1). To further explore this, additional modeling has been completed on "System A" and on a number of other random systems.

Revisiting System A

The fully defined six unit process system from Section 4.1 was used again to demonstrate convergence of the mean after 2000 iterations of the Monte Carlo Analysis. Figures 4.6, 4.7, and 4.8 show the relationship of the mean CO_2 output to the number of iterations. Each of the three runs of System A resulted in a different (random) path towards clear convergence after 1000 iterations.

Testing Convergence on Larger Systems

It is important to know whether LCA system size and complexity affects the rate of Monte Carlo Analysis convergence. To test this, three randomly generated systems were used, each made up of 50 unit processes. Each system was run for 4000 iterations. The cumulative mean plotted against the number of iterations for these three systems is shown in Figures 4.9, 4.10, and 4.11. As seen by the plots, each system converged by 2000 iterations. The mean acquired through Monte Carlo Analysis at convergence, compared to the known mean was within 0.5% for each system.



Figure 4.6: Convergence of Mean for System A – Test 1



System A - Convergence of Mean - Test 2

Figure 4.7: Convergence of Mean for System A – Test 2

1 10 100 1000 10000 Number of Iterations

System A - Convergence of Mean - Test 3

Figure 4.8: Convergence of Mean for System A – Test 3



Figure 4.9: Convergence of Mean for Random System 1



Figure 4.10: Convergence of Mean for Random System 101



Figure 4.11: Convergence of Mean for Random System 201

4.3 – Non-Linearity in Modeling LCA Systems

In general, LCA involves the modeling of linear systems. In other words, the total environmental output is assumed to be linearly related to each data point. Normally, a LCA system is made up of a collection of unit processes, each of which produces environmental outputs governed by a linear relationship to the process's products and inputs. As a simple example, consider "System A" from Section 4.1 (repeated below in Figure 4.12). The governing equation of the total environmental outputs of System A is the linear function shown in equation 4.4.



Notes: P_k = flow of a product or service e.g. steel, power, etc.

 x_{ij} = environmental output of type "j" from unit process "i".

Figure 4.12: Process Flow Diagram for the Fully Defined LCA System, "System A" (From 4.1)

Total Emissions = $X = f(F_{nu}, P_1, P_2, P_3, P_4, P_5, P_6, I_{12}, I_{24}, I_{25}, I_{13}, I_{36}, x_{11}, x_{21}, x_{31}, x_{41}, x_{51}, x_{61})$

$$X = f = \frac{P_{F_n}}{P_1} \left[x_{11} + \frac{I_{12}}{P_2} \left(x_{21} + \frac{I_{24}}{P_4} x_{41} + \frac{I_{25}}{P_5} x_{51} \right) + \frac{I_{13}}{P_3} \left(x_{31} + \frac{I_{36}}{P_6} x_{61} \right) \right]$$

Note: P_{Fn} = Functional Unit; I_{ij} = Input to unit process "i" from unit process "j".

Figures 4.13, 4.14, and 4.15 show the linear relationship between various parameters (I12, x11, and x21) and the total environmental output. The slope of these lines provide an indication of the sensitivity of the results to each parameter. Knowledge of this

(4.4)

sensitivity enables one to identify which unit processes have the greatest impact on the overall results and indicates which unit processes to focus on for collecting higher quality data. In this example, the total environmental output is shown to change quite rapidly with changes in I12 as shown in Figure 4.13. Analytically, one can calculate the relative sensitivity of each parameter using the first derivative of the governing equation. However, with larger, more complex systems, this becomes extremely burdensome. As a result, a numerical method of estimating relative sensitivity is desirable.



Figure 4.13: Relationship Between Input to UP1 from UP2 and Total Environmental Output for System A



Figure 4.14: Relationship Between Environmental Output from Unit Process UP1 and Total Environmental Output for System A



Figure 4.15: Relationship Between Environmental Output from Unit Process UP2 and Total Environmental Output for System A

A numerical approach to assessing sensitivity is presented by RAYNOLDS *et al* [1] where each parameter in the system is independently given a marginal change to calculate the marginal impact on the overall results. A similar method has been applied to System A with the results shown in Tables 4.5 and 4.6. The Tables show that a 1% increase in the inputs required for unit process UP1 results in a 0.84% increase in total environmental output. Of all the unit processes in the system, UP1 generates the greatest sensitivity. Next most sensitive is the environmental output data for unit process UP2, where a 1% increase in emissions from UP2 resulted in a 0.57% increase in System A's total environmental output.

 Table 4.5:
 Marginal Sensitivity of Unit Process Inputs for System A

	Marginal Change (%) in Total Environmental Output Due to 1% Increase in Input Requirements to Individual Unit Processes					
Stressor Category	UP1	UP2	UP3	UP4	UP5	UP6
Greenhouse Gases	+0.84	+0.21	+0.03	0	0	0

 Table 4.6:
 Marginal Sensitivity of Unit Process Emissions for System A

	Marginal Change (%) in Total Environmental Output Due to 1% Increase in Individual Unit Process Environmental Outputs					
Stressor Category	UP1	UP2	UP3	UP4	UP5	UP6
Greenhouse Gases	+0.16	+0.57	+0.03	+0.13	+0.07	+0.03

As shown in Table 4.4 of Section 4.1, using Monte Carlo Analysis repeatedly, the overall uncertainty of results for System A is highly dependent on unit process UP1 and slightly dependent on unit process UP2.

Having identified the unit processes with the greatest sensitivity on the overall results, the question to answer is how the results will change if a non-linearity is introduced to one of these sensitive unit processes. This is where the flexibility of Monte Carlo Analysis becomes extremely useful as analytically evaluating these systems would quickly become burdensome.

Sources of Non-Linearity

There are two primary means by which non-linearity can enter a LCA system:

- 1. The relationship between environmental outputs, inputs and product outputs of any unit process becomes non-linear. This can occur due to change in performance over time (e.g. emissions from a vehicle as it ages), scale of operation (e.g. the input-output relationship changes with the scale of the operation), or non-linear physical relationships (e.g. fuel efficiency of a vehicle at different speeds). Evaluating the overall uncertainty of systems with non-linear unit processes is possible with the techniques of Monte Carlo Analysis developed here.
- 2. The distribution of uncertainty for any given data point is non-normal, that is a skewed distribution. The question is when will a skewed distribution affect the overall results? This will depend on the sensitivity of the unit process with the skewed distribution. Monte Carlo Analysis enables one to model data with a skewed distribution, a task which analytically would be very difficult.

Applying a Skewed Distribution to System A

To test the impact of a skewed distribution for unit process input and output data, a beta distribution was applied to different unit processes in System A.

Two different beta distributions (B(α , β)) were used: B(1,5) and B(2,5). Figures 4.16 and 4.17 illustrate these two beta distributions in comparison to the normal distribution with equivalent standard deviations.
Beta (1,5) vs Normal (+/- \$5.2%)



Figure 4.16: Comparison of the Beta Distribution (1,5) to the Normal Distribution with Equal Standard Deviations



Figure 4.17: Comparison of the Beta Distribution (2,5) to the Normal Distribution with Equal Standard Deviations

Both beta distributions were applied to different unit processes in System A to asses their overall impact on the distribution of uncertainty for the total environmental output of System A. Figures 4.18 and 4.19 show the results of the distribution of uncertainty for System A when:

- 1) all unit processes have a normal distribution of uncertainty,
- 2) all unit processes have a beta distribution of uncertainty,
- 3) unit process UP1 has a beta distribution,
- 4) unit process UP2 has a beta distribution, and
- 5) unit process UP3 has a beta distribution.

For each run the mean value is held constant. The results show the skewed distribution to significantly affect the spread of uncertainty when applied to the sensitive unit processes – UP1 and UP2. When applied to unit process UP3, the overall distribution is not significantly affected. It is clear the distribution can affect the end decision. Should the distribution be skewed with a large uncertainty, the level of confidence in decision making will be reduced. The use of Monte Carlo Analysis to assess the propagation of error throughout systems in LCA is very effective, especially when unit processes have skewed uncertainty distributions. Further research in the field of LCA is required to better address how to obtain distribution functions for individual data points.



Figure 4.18: Comparison of the Distribution of the Total Environmental Output of System A for Normal Distribution and Various Applications of the Beta B(1,5) Distribution



Figure 4.19: Comparison of the Distribution of the Total Environmental Output of System A for Normal Distribution and Various Applications of the Beta B(2,5) Distribution

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Chapter 5

Integrating the System Boundary and Uncertainty Analysis Tools into the Inventory Assessment Stage of LCA

Chapter 5 presents the collection of individual tools presented in Chapters 2 through 4 into an integrated package fitting into the Inventory Assessment stage of LCA.

5.0 – Integrating the System Boundary and Uncertainty Tools into the LCA Methodology

The tools presented in chapters two through four can be applied sequentially to provide a practical and rigorous methodology for completing the life-cycle inventory (LCI) stage of life-cycle assessment (LCA). This chapter summarizes each tool and describes where they fit into the LCA methodology.

The RMEE method of system boundary ensures similar boundaries are selected for different systems. It provides an indication of when enough detail has been included in the system to make a reasonable decision without first having to calculate all the environmental outputs of each system. The RMEE method is designed for LCA studies of energy and material systems where common combustion emissions are being quantified for comparison. Marginal sensitivity analysis shows which data points have the greatest influence on the mean results, indicating early on in the LCI where to focus data collection. Monte Carlo Analysis provides an efficient means to estimate the overall propagation of uncertainty. Applied iteratively (systematically removing unit process uncertainty), Monte Carlo Analysis is used to identify which unit processes in the lifecycle system contribute the most to uncertainty. This tool for assessing the benefit of reducing uncertainty in different unit processes has been called "Uncertainty Reduction Analysis". It focuses data research on the specific unit processes contributing the most to the overall uncertainty in the decision. Applying Monte Carlo Analysis to combine overall uncertainty in data with uncertainty associated with the system boundary provides a practical method to estimate total uncertainty for each system. The results enable one to numerically calculate the probability one system results in less potential environmental impact than another.

Chapter 1 presented the general LCA methodology (refer to Figure 5.1). Figure 5.2 illustrates how each tool developed by this research fits into the Inventory Assessment stage of LCA.

The Goal Definition and Scoping step of LCA are unaffected by the tools. This first step must provide a functional unit and a qualitative process flow map of each life-cycle system. The package of tools fit into the Inventory Assessment phase of LCA. Together they help minimize the time and effort required to obtain enough information to make a confident decision between two or more options.

The inventory assessment becomes a process of iteratively collecting better quality data as required. First, (Step 1) initial material, energy and value input and output flow data are collected for the initial life-cycle process flow map defined in the Goal and Scope Definition. These data are used to select an initial system boundary defined by the Z-Cut-off-Ratio in the RMEE method (Step 2). The RMEE method indicates for which unit processes environmental output data is required (Step 3). With complete data on the inputs, outputs, and environmental outputs for all unit processes, marginal sensitivity analysis is completed to identify which unit processes in the system create the greatest sensitivity in the results (Step 4). The practitioner can then focus data research efforts on these sensitive unit processes.

After calculating or estimating uncertainty for each input and environmental output in each unit process, the total uncertainty due to data, for each system, is calculated using the Monte Carlo Analysis technique (**Step 5**). This uncertainty (r_{Data}) and the uncertainty derived from the RMEE method ($r_{SysBndry}$) are combined to provide an estimate of the total system uncertainty (r_{Total}). Monte Carlo Analysis is used to combine r_{Data} and $r_{SysBndry}$ to calculate r_{Total} (**Step 6**).

Using the mean emissions output and total system uncertainty (r_{Total}) for both systems being compared, the probability or confidence of one system resulting in less emissions of each environmental stressor category is calculated (Step 7). With the mean and uncertainty for each option plus a prescribed level of confidence that one system will produce less emissions than another, the LCA practitioner must decide if the results allow for decision making (Step 8). If so, the practitioner proceeds to the impact analysis and interpretation phases of LCA. If the results do not allow the decision maker to conclude which option is best with an acceptable level of certainty, then Uncertainty Reduction Analysis is completed to identify the best options for reducing overall uncertainty (Step 9).

The Uncertainty Reduction Analysis will identify how the overall uncertainty can be reduced. The decision maker uses the results and considers how much time and resources are available to improve data quality or expand the system boundaries in order to make a better decision (Step 10). If the decision is made to invest more time and resources, two things can be completed together or separately to reduce the uncertainty:

- collect better data on the unit processes identified by the Uncertainty Reduction Analysis to have the greatest potential for reducing uncertainty due to data (Step 11) and/or,
- increase the coverage of the system boundary by reducing the Z-Cut-off-Ratio (Step 12) which will reduce the uncertainty introduced due to system boundary selection.

Both steps 11 and 12 result in re-iterating parts of the inventory assessment and may be repeated until a confident decision can be made. However, the decision maker may decide at Step 10 that no additional time and resources are available for collecting additional information. Two options are then available:

- return to the Goal and Scope Definition to reframe the decision to be made into one which can be answered by the results; or
- 2) accept the information generated so far, be conscious of the uncertainty and proceed to impact assessment and interpretation in order to make a decision.

This package of tools, designed and developed to streamline the LCI stage of LCA, results in a repeatable and quantitative method for completing LCA. Understanding the level of confidence one has using LCI results to make decisions should improve the quality of those decisions and illustrate the need to improve the quality of LCA studies. The next chapter presents a case study applying this systematic method of Inventory Assessment (LCI).



Figure 5.1: LCA Methodology

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Figure 5.2: Integration of Streamlining Tools into the Inventory Assessment stage of LCA

Chapter 6

A Case Study Life-Cycle Assessment (LCA) Applying the Relative Mass-Energy-Economic (RMEE) Method of System Boundary Selection and Monte Carlo Analysis to Automotive Fuels

It is the purpose of Chapter 6 to demonstrate the integrated set of tools presented by this thesis. Chapter 6 is a paper, which will be submitted to the International Journal of Life-cycle Assessment. It utilizes the tools summarized in Chapter 5 to evaluate the life-cycle environmental inventory of three different automotive fuels: reformulated gasoline, natural gas, and 85% blended ethanol (E85).

6.1 Introduction

Canada's commitment to reduce greenhouse gases has brought significant attention to all sectors of the economy using fossil fuels – the major source of anthropogenic carbon dioxide emissions. In Canada, the transportation sector emits 27% of the nation's total greenhouse gases, of which over 60% is the result of gasoline combustion [13]. Canada has alternative fuels with the potential to reduce CO₂ emissions per kilometer driven. To properly compare fuel options, the production of the fuel must be considered from raw material acquisition through processing to final use of the fuel – i.e. the "life-cycle" of the fuel. The objective of this work is to compare the relative performance of three different automotive fuels based on a life-cycle assessment (LCA) approach. The fuels considered are reformulated gasoline, natural gas, and E85 (85% ethanol, 15% gasoline). For the reformulated gasoline systems, crude oil is assumed to be derived from oil sands operations in northern Alberta. Crude oil from oil sands is Alberta's rapidly growing marginal source of crude but does not represent the industry average. For E85, two sources of ethanol are considered - corn and poplar trees. Each fuel is considered based on production and consumption in Canada. Because local air quality is of particular concern in a number of Canadian cities, ground level ozone precursors and acid rain precursors are also compared for each fuel.

The primary purpose of this paper is to demonstrate the use of specific LCA tools for system boundary selection and uncertainty analysis on a comparison of automotive fuels. This paper completes the first two steps of LCA – 1. goal definition and scoping, and 2. inventory assessment, but does not complete 3. impact analysis, or 4. interpretation. The primary objective of this paper is to demonstrate the tools developed by *Raynolds et al* [17][18][19].

6.2 The RMEE Method of System Boundary Selection and Tools for Uncertainty Analysis

RAYNOLDS et al [18][17][19] have developed LCA tools for selecting system boundaries and evaluating uncertainty. These have been combined to create a logical method of identifying if and where time and resources should be expended to reduce uncertainty in the results. This method incorporates the RMEE method for system boundary selection as well as Monte Carlo Analysis to provide a rigorous, and quantitative method for selecting system boundaries and assessing overall data uncertainty. The Uncertainty Reduction Analysis tool [17] is also incorporated to quantify the potential reductions in overall uncertainty. Figure 6.1 illustrates the combination of these tools.



Figure 6.1: Inventory Analysis Tools

6.3 The Automotive Fuel Case Study

6.3.1 Goal Definition

Purpose

The purpose of this LCA is to:

- 1. Demonstrate the use of recent advancements in LCA including the Relative-Mass-Energy-Economic (RMEE) method of system boundary selection, marginal sensitivity analysis, Monte Carlo Uncertainty analysis, and Uncertainty Reduction Analysis.
- 2. Compare the relative environmental performance of MTBE reformulated gasoline, ethanol blended gasoline (E85), and natural gas over the life-cycle of each fuel from raw material acquisition through to combustion in a light-duty passenger vehicle. Each fuel is produced and used in Canada.

System Options

Numerous fuel options exist for passenger vehicle fuels. Options not considered by this LCA include hydrogen for fuel cells, electricity, propane, diesel and methanol. (All of these could be compared in a more extensive study using the methodology presented by this work.) The fuel systems selected for this analysis are considered to be available today on a commercial scale (except for ethanol from poplar trees which is currently at pilot scale). Table 6.1 describes the systems compared by this LCA.

System Name	Final Fuel	Upstream Source(s)	Notes
RFG	MTBE Reformulated Gasoline	Oil Sands Crude	15% MTBE, 85% gasoline
CNG	Natural Gas	Alberta Average	
E85-Corn	Ethanol Blended Gasoline (E85)	Oil Sands Crude /Corn Ethanol	Corn ethanol production occurs in Ontario
E85-Poplar	Ethanol Blended Gasoline (E85)	Oil Sands Crude / Poplar Ethanol	Commercial scale operation does not yet exist in Canada.

 Table 6.1:
 Fuel Systems Analyzed by this LCA

Assumptions and Limitations

The life-cycle of fuel systems is very complex. It is important to recognize that like any LCA, this analysis has a number of limitations and has required certain assumptions. The assumptions and limitations of this work include:

- This analysis provides a relative comparison between fuel options for the purpose of decision making. The numbers presented should not be interpreted as the 'absolute' values for the life-cycle of each fuel.
- There has been no economic analysis. This work is limited to an environmental comparison.
- The data values used in this analysis are all from publicly available data sources.
- No tracking of the geographical location of environmental outputs has been completed. That is, the sum of all emissions for each stressor category is presented. This is important for ground level ozone precursors and acid rain precursors which are stressor categories having regional specific impacts.
- No future technology analysis has been completed. This analysis takes a snapshot of current technology and does not attempt to predict process or performance improvements over time.
- The implications of wide-scale use of each fuel have not been considered. This is especially important for E85 which is unlikely to be capable of supplying the entire Canadian fleet's fuel demand. This study considers marginal growth opposed to supply to the of the entire industry.

Audience

This work is primarily intended to demonstrate the use of RMEE and Monte Carlo Analysis to practitioners of LCA. The secondary audience is the fuel industry and public policy makers interested in the relative environmental performance of different automotive fuels available in Canada.

Time and Resources

This work has been completed by one primary researcher working part time over a five month period with approximately 160 person hours available for completion.

6.3.2 Scope Definition

Functional Unit

The functional unit is defined as the quantity of fuel required to travel 1000 km in a lightduty passenger vehicle in an urban setting. Fuel consumption rate is based the U.S. FTP Urban test cycle [23].

Process Flow Diagrams

The process flow diagrams presented in Figures 6.2, 6.3, 6.4 and 6.5 illustrate the four fuel systems being compared. The dotted line represents the system boundary as defined by the Relative Mass-Energy-Economic method at $Z_{RMEE}=0.15$ (see "System Boundary Selection" below).







Process flow diagram for the compressed natural gas (CNG) System Figure 6.3:









Environmental Stressor Categories

Table 6.2 lists the environmental stressor categories quantified by this LCA and the factors applied to contributing pollutants. This LCA focuses on common combustion emissions. Generally this process of lumping emissions using relative factors to give environmental stressor categories is completed in the Impact Analysis step of LCA [22]. However, since this process is generally a numerical process, here it is included in the Inventory Assessment stage of LCA. This makes it easy to apply uncertainty analysis to the stressor categories on which a decision will be based.

Stressor Category	Units	Contributing Pollutants [24]	Reason for Inclusion
Greenhouse Gases (GHG)	kg CO ₂ Equivalents	$\frac{1 \times CO_2 + 21 \times CH_4 + 320}{\times N_2O}$	International commitments to reducing GHG emissions.
Acid Rain Precursors (ARP)	kg SO ₂ Equivalents	$1 \times SO_2 + 0.70 \times NOx$	Concern in certain regions of Canada due to acidification of water bodies.
Ground Level Ozone Precursors (GLO)	kg NOx + VOCs	1 x NOx + 1 x VOCs (volatile organic combounds)	Concern for urban areas due to smog and respiratory impacts.

 Table 6.2:
 Environmental Stressor Categories

Numerous other environmental stressor categories exist and could be quantified for a more complete environmental comparison between fuel options, (e.g. particulate matter, water pollution, hazardous air pollutants, etc.). However, due to data limitations, quantification of all these stressor categories was not possible. Emphasis has been placed on air pollutants as this is the direct and major impact of fuel use. It must be emphasized that the primary purpose of this work is to demonstrate the use of the RMEE boundary selection and uncertainty analysis tools.

6.3.3 Inventory Assessment

System Boundary Selection

The first step in the inventory assessment stage is to select the system boundary. The Relative Mass-Energy-Economic (RMEE) method of system boundary selection requires collection of material and energy flow data but does not require environmental output data (Figure 6.1 – Step 1) [17]. The RMEE method has been applied with a Z_{RMEE} cut-

off ratio of 0.15 (Figure 6.1 – Step 2) [18][17]. Prior research shows this will give comparable results for all systems at an uncertainty level of approximately 30% [17]. The resulting system boundaries are presented in the process flow maps in Figures 6.2 through 6.5.

For the purpose of running RMEE, the mass, economic and energy value of the functional unit is measured based on the fuel required to provide the 1000 km distance of travel. Table 6.3 shows the values used for the functional unit of each system for completing the RMEE evaluation.

System	Amount	Mass (kg)	Energy (MJ)	Economic (\$)
RFG	116 liter	87	3710	67.19
CNG	135 m ³	88	4490	10.13
E85	153 liter	119	3245	88.87

 Table 6.3:
 RMEE Values for Functional Unit of Each System

With the Z_{RMEE} cut-off ratio at $Z_{RMEE} = 0.15$, the manufacture of the vehicle should be included due to its cost. However, because the purpose of this LCA is to present a relative comparison between options and the environmental outputs associated with manufacturing each vehicle type are approximately equal, the upstream unit processes involved in manufacturing the vehicle are eliminated from the analysis. They would not change the decision making. Similar assumptions have been made for upstream impacts from vehicle maintenance.

Allocation Method

It is important to document the method used in the allocation of unit process inputs and environmental outputs between the main product and the co-products that are simultaneously produced. Here, allocation of environmental outputs and unit process inputs to products is completed by market value allocation.

Data Sources

Tables 6.4 through 6.8 summarize the data sources used to collect environmental output data (Figure 6.1: Step 3) for this LCA. Appendix III provides a print-out of each data set used in the model.

Unit Process / Data Set	Data Sources	Notes
Produce Crude Oil / Aggregated - Syncrude Suncor Monenco	[4] [21] [10]	All three data sources were combined using a t-distribution to obtain aggregated data set.
Refinery / Shell Scotford 1993	[20]	Plant is designed for oil sands crude oil. Allocation of outputs based on average of mass, energy and economic value (all within one percentage point.)
Transport Crude Oil / Monenco 1992	[10]	
Produce Alberta Electricity / Average Integrated System 1995	[22]	Represents Alberta average grid consisting of 89% coal power, 8% natural gas power, and 3% from hydro power.
Produce Natural Gas / Monenco 1992 Aggregated	[10]	
Transmit Electricity / Grid Average	[22]	Grid average loss is 7% due to transmission.
Transport Natural Gas / Nova Gas 1996	[14]	
Transport Fuel / Diesel Truck – 50km	[7]	Assumes a 50km distance from refinery to filling station. The assumption for this example is the fuel is consumed within a 50km radius of the refinery.

 Table 6.4:
 Data Sources for Unit Processes Common to More than one System

Table 6.5: Data Sources for RFG System

Unit Process / Data Set	Data Source	Notes
Operate Vehicle / RFG – Taurus - 1995	[11]	Based on average and statistics of actual measured data of in-use U.S. Federal fleet vehicles.
Produce MTBE / Aggregated – EnviroFuels, ABC	[2] [1]	Data sources were combined using a t-distribution to obtain aggregated data set.
Produce Methanol / Methanex 1997	[9]	
Transport MTBE / Diesel Truck 1000km	[7]	Assumes MTBE is transported 1000 km to the blending facility.
Refuel Vehicle / RFG	[5]	Includes all emissions from service station operations.

Table 6.6: Data Sources for CNG System

Unit Process / Data Set	Data Source	Notes
Operate Vehicle / Natural Gas – Taurus – Conversion - 1994	[11]	Based on average and statistics of actual measured data of in-use U.S. Federal fleet vehicles. These vehicles are CNG conversions.

Table 0.7: Data Su	TICES IVI EO	5-CULI SASIEII
Unit Process / Data Set	Data Source	Notes
Operate Vehicle / E85 – Taurus – NREL - 1995	[11]	Based on average and statistics of actual measured data of in-use U.S. Federal fleet vehicles.
Produce Ethanol / Commercial Alcohols - Chattam	[6]	Input and output data used to calculate emissions from natural gas combustion. Allocation of co-products allocated based on market value.
Produce Corn / Ontario	[3]	Mean harvest of 6,660 kg per hectare applied.
Transport Corn / Diesel Truck – 60km	[7]	Assume corn is transported 60km to facility. It is assumed the ethanol plant is located in a corn-farming area i.e. southern Ontario.
Transport Ethanol / Ontario – 3000km - Rail	[7]	Assume ethanol is transported 3000 km to refinery from ethanol facility. The assumption is corn-ethanol, produced in Ontario, is transported to the refinery located in Alberta.
Refuel Vehicle / E85	[5]	Data is for gasoline and therefore is not representative of E85.
Produce Electricity – Ontario / Ontario Hydro 1996 - Coal	[16]	
Transport Natural Gas to Ontario / 3000km Nova Gas 1996	[14]	

 Table 6.7:
 Data Sources for E85-Corn System

Table 6.8: Data Sources for E85-Poplar System

Unit Process / Data Set	Data Source	Notes
Operate Vehicle / E85 – Taurus – NREL - 1995	[11]	Based on average and statistics of actual measured data of in-use U.S. Federal fleet vehicles.
Produce Ethanol / Enzymatic - NREL 1998 - AB Elec Credit	[12]	Assume electricity produced by the ethanol production system offsets average Alberta grid electricity.
Produce Poplar / NREL 1997 – Drayton Valley Region	[15]	Harvesting yields based on Alberta farmer experience.
Transport Ethanol / Ethanol – 300km - Truck	[7]	Assumes ethanol is transported 300km to blending. The assumption is the ethanol facility will be located in an area suitable for poplar plantations and is assumed to be located 300 km from the fuel blending facility.
Transport Poplar / Diesel Truck – 60km	[7]	Assumes poplar is harvested within 60km radius of ethanol plant.
Refuel Vehicle / E85	[5]	Data is for gasoline and therefore is not representative of E85.

Known Data Gaps

The following are known data gaps in this analysis:

- Data not available on the release of emissions from soil in growing and fertilizing corn crops and poplar trees. If data were available it would increase the GHG emissions of the E85-corn system but would have a very minor impact on the E85-poplar system since very little fertilizer is used in poplar plantations.
- Available data on refueling vehicles with different fuels was not readily available. As a result the emissions have been considered comparable for all liquid fuels.
- Leakage rates from natural gas vehicles are unknown.

Mean Results and Marginal Sensitivity Analysis

Following system boundary selection and the collection of environmental output data (Figure 6.1 -Steps 2 and 3), each system was modeled to calculate the mean results of each stressor category (Figure 6.1 -Step 4). Additionally, marginal sensitivity analysis was run on each system in order to identify the unit processes having the most significant impact on the final results (Figure 6.1 -Step 4)[refer to Section 4.4 of thesis]. Each unit process of each system was tested for its sensitivity to a 1% decrease in input/product "efficiency" ratio, and a 1% increase of emissions outputs/products ratio. A data point for a unit process is considered to be significant if its marginal sensitivity on the total system output of a stressor category is greater than 0.25%. This means if a 1% change in a single unit process ratio changes the total system value of a stressor category by 0.25% then that data point significantly affects the conclusions of the analysis.

Tables 6.9 through 6.23 show the mean results, the input flow sensitivity, and the emissions sensitivity for each system.

Tables 6.9 through 6.12 cover the RFG system. Table 6.9 presents the mean environmental output results for greenhouse gases, acid rain precursors and ground level ozone precursors for each unit process in the system. Table 6.10 shows the marginal sensitivity of the input to product ratio for the most significant unit processes in the system. Table 6.11 shows the marginal sensitivity of the environmental output to product ratio for each unit process. The marginal sensitivity analysis shows the RFG system is most sensitive to the values shown in Table 6.12. The RFG system is most sensitive to three unit processes: Produce Crude Oil, Operate Vehicle, and the Refinery. All three of these data sets are from the best known available sources of data.

Tables 6.13 through 6.16 cover the CNG system. Table 6.13 presents the mean environmental output results for each stressor category. Table 6.14 shows the marginal sensitivity of the input to product ratio for the most significant unit processes in the system. Table 6.15 shows the marginal sensitivity of the environmental output to product ratio for each unit process. For the CNG system, the marginal sensitivity analysis shows the system to be most sensitive to the values shown in Table 6.16. The CNG system is most sensitive to two unit processes: Operate Vehicle, and Produce Natural Gas. Both of these data sets are from the best known available sources of data.

Tables 6.17 through 6.20 cover the mean and sensitivity results for the E85-Corn system. Table 6.17 shows the mean environmental output results for the three environmental stressor categories. Table 6.18 shows the marginal sensitivity of the input to product ratio for the most significant unit processes in the system. Table 6.19 shows the marginal sensitivity of the environmental output to product ratio for each unit process. Marginal sensitivity analysis of the E85-Corn system indicates the results are most sensitive to the values shown in Table 6.20. The results are most sensitive to four unit processes: Operate Vehicle, Produce Ethanol, Produce Crude Oil, and Transport Natural Gas. All four of these data sets are from the best known available sources of data.

Tables 6.21 through 6.24 cover the mean and sensitivity results for the E85-Poplar system. As the mean results presented in Table 6.21 show, the production of ethanol from poplar results in an actual reduction of environmental outputs. This is because the enzymatic process of producing ethanol from biomass results in the production of both ethanol fuel and electricity. In this analysis it is assumed the electricity produced by the ethanol plant offsets average Alberta grid electricity since the plant would be operated in Alberta. Because the ethanol plant requires no fossil fuel inputs, its stack emissions are relatively low. When subtracting the emissions, which would result if the same amount

of electricity were produced by the average grid, the net change in overall emissions is negative. Table 6.22 shows the marginal sensitivity of the input to product ratio for the most significant unit processes in the system. Table 6.23 shows the marginal sensitivity of the environmental output to product ratio for each unit process.

The marginal sensitivity analysis for the E85-Poplar system indicates the results to be most sensitive to the values shown in Table 6.24. The E85-Poplar system is most sensitive to six unit processes: Operate Vehicle, Produce Ethanol, Produce Poplar, Refinery, Produce Crude Oil, and Refuel Vehicle. Except for the Refuel Vehicle unit process, all data points are from best available data. However, it must be emphasized that there is greater uncertainty in the Produce Poplar and Produce Ethanol processes than in comparable processes for present commercial fuels.

Because the baseline results of greenhouse gases and acid rain precursors are negative values it is important to understand what a negative or positive sensitivity means. As an example, consider the sensitivity of the fuel requirements for operating the vehicle where a 1% increase in fuel requirements results in a 1.5% change in the total emissions of greenhouse gases (from -102.71 to -104.25 kg CO₂ Equiv). This is a counter-intuitive result – consuming more fuel results in **less** emissions. The reason is that the production of fuel offsets average grid electricity because the cellulose ethanol plant is a cogeneration system (shown in Figure 6.5). The offset electricity has a high greenhouse gas intensity resulting in significant reductions in emissions. So, the more fuel consumed the greater the amount of electricity offset, the greater the reduction in greenhouse gas emissions. Of course this is only true when considering a marginal fuel production rate and would not be valid at a scale where the production of electricity from ethanol plants significantly changes the average grid electricity.

Consider the sensitivity of the emissions of the "Produce Ethanol" unit process where a 1% increase in the greenhouse gas offset generated by the plant results in a 2.01% change in the total greenhouse gases (from -102.71 to -104.77 kg CO₂ Equiv.). The interpretation here is the 1% increase in offsets generated at the ethanol plant results in an overall 2.01% increase in the total offset. The results are very sensitive to the Produce Ethanol unit process and the assumption of its electricity offsetting grid average power.

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Table 6.9: Mean Results of RFG System

Stressor	Units	Total	Produce	Transport	Produce	Refinery	Transport	Refuel	Operate
Category		-	MTBE	MTBE	Crude Oil		Fuel	Vehicle	Vehicle
Greenhouse Gases	kg CO ₂ Equiv.	395.59	5.47	1.56	97.18	25.32	0.52	0.00	265.54
	%	100	1.38	0.39	24.57	6.40	0.13	0.00	67.13
Acid Rain	kg SO ₂ Equiv.	1.35	0.00	0.00	1.26	0.02	0.00	0.00	0.06
	%	100	0.34	0.34	93.59	1.27	0.11	0.00	4.35
Ground Level Ozone	kg NOx + VOC	0.62	10.0	0.01	0.24	0.08	0.00	0.12	0.17
	%	100	1.12	1.23	38.69	12.35	0.41	18.94	27.25

Marginal Sensitivity of Input to Product Ratio for Significant Unit Processes in the RFG System (1% increase in input required to produce same product) **Table 6.10:**

	(1 70 Increase in input required to produ	ndui ui	Lednice	a to proat
Stressor	Units	Baseline	Baseline Refinery Operate Vehicle	Operate Vehicle
Greenhouse Gases	kg CO2 Equiv.	395.59	0.25 %	395.59 0.25 % 0.33 %
Acid Rain Precursors	kg SO2 Equiv.	1.35	0.94 %	1.35 0.94 % 0.96 %
Ground Level Ozone	Ground Level kg NOx + VOC Ozone	0.62	% 6£.0	0.62 0.39 % 0.73 %

	(1% increase	in enviror	nmental or	tputs to p	case in environmental outputs to produce same product)	: produc	()		
Stressor	Units	Baseline		Transport	Transport Produce Crude Refinery Transport	Refinery	Transport	Refuel	Operate
			MTBE	MTBE	Oil		Fuel	Vchicle	Vehicle
Greenhouse	kg CO2 Equiv.	395.59	0.01 %	0.00 %		0.25 % 0.06 %	0.00 %	0.00 %	0.67 %
Gases									
Acid Rain	kg SO2 Equiv.	1.35	% 00.0	0.00 %		0.94 % 0.01 %	0.00 %	00.0	0.04 %
Precursors									
Ground Level k kg NOx +	k kg NOx +	0.62	0.01 %	% 10.0		0.39 % 0.12 %	00.0	0.19 %	0.27 %
Ozone	voc								

 Table 6.11:
 Marginal Sensitivity of Environmental Output to Product Ratio for Each Unit Process in the RFG System

Table 6.12: Identification of Unit Process Data Points with Significant (>0.25%) Sensitivity in the RFG System

	D	D
Unit Process	Sensitivity of Input Data to	Sensitivity of
	Stressor Categories	Environmental Output
		Data to Stressor Categories
Produce Crude Oil	Inputs to crude oil production	- ARP (0.94)
	outside system boundary.	- GLO (0.39)
		- GHG (0.25)
Operate Vehicle	Fuel requirements:	- GHG (0.67)
	- ARP (0.96)	- GLO (0.27)
	- GLO (0.73)	
	- GHG (0.33)	
Refinery	Crude oil requirements:	Not sensitive.
	- ARP (0.94)	
	- GLO (0.39)	
	- GHG (0.25)	

CNG System

Table 6.13: Mean Results of CNG System

Stressor	Units	lotal	l'roduce	I ransport	Ketuel	Operate
Category			Natural Gas	Natural Gas	Vehicle	Vehicle
Greenhouse Gases	kg CO ₂ Equiv.	337.23	39.65	30.56	18.56	248.46
	%	100	11.76	9.06	5.50	73.68
Acid Rain Precursors	kg SO ₂ Equiv.	0.83	0.43	0.15	0.00	0.26
	%	100	51.07	18.17	0.00	30.75
Ground Level Ozone	kg NOx + VOC	0.92	0.31	0.22	0.00	0.39
	%	100	34.13	23.58	0.00	42.29

Table 6.14: Marginal Sensitivity of Input to Product Ratio for Significant Unit Processes in the CNG System (1% increase in input required to produce same product)

	TT /0 IIICI CAN	(1 /0 mercase in mbar redamen to br	d on no linh
Stressor	Units	Bascline	Operate Vehicle
Greenhouse Gases	Greenhouse kg CO2 Equiv. Gases	337.23	0.26 %
Acid Rain Precursors	kg SO2 Equiv	0.83	0.69 %
Ground Level Ozone	Ground Level kg NOx + VOC Ozone	0.92	0.58 %

	(1% increase	in environn	(1% increase in environmental outputs to produce same product)	s to produce	e same pro	duct)
Stressor	Units	Baseline	Produce	Transport	Rcfucl	Operate
			Natural Gas	Natural Gas	Vehicle	Vehicle
Greenhouse	Greenhouse kg CO2 Equiv.	337.23	0.12 %	0.09 %	0.06 %	0.74 %
Gases						
Acid Rain	kg SO2 Equiv	0.83	0.51 %	0.18%	0.00 %	% 16.0
Precursors						
Ground Level	Ground Level kg NOx + VOC	0.92	0.34 %		0.24 % 0.00 %	0.42 %
Ozone						

Table 6.15: Marginal Sensitivity of Environmental Outputs to Product Ratio for Each Unit Process in the CNG System

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Table 6.16: Identification of Unit Process Data Points with Significant (>0.25%) Sensitivity in the CNG System

TADIC O'LO: TACIM	I ADIC 0.10: TUCHINICATION OF OTHE LEOCOSS DATA FOILD WITH ORDINICAU	LA FUIRIS WILL DIGHTICAR	
Unit Process	Sensitivity of Input Data to	Sensitivity of	
	Stressor Categories	Environmental Output	
		Data to Stressor Categories	
Operate Vehicle	Fuel requirements:	- GHG (0.74)	
	- ARP (0.69)	- ARP (0.31)	
	- GLO (0.58)	- GLO (0.42)	_
	- GHG (0.26)		
Produce Natural Gas	Inputs upstream of producing	- ARP (0.51)	
	natural gas are outside	- GLO (0.34)	
	system boundary.		

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Stressor	Units	Total	Produce	Transport	Produce	Transport	Produce	Transport	Produce	Refinery	Transport	Refuel	Operate
Category			Natural	Natural	Com +	Com	Ethanol	Ethanol	Crude Oil		Fuel	Vehicle	Vchicle
			Gas	Gas	Storage								
Greenhouse	kg CO ₂	224.7	9.68	44.75	10.70	1.14	70.61	7.26	22.69	5.91	0.65	0.00	51.28
Gases	Equiv.												
	%	001	4.31	19.92	4.76	0.51	31.43	3.23	10.10	2.63	0.29	00.0	22.83
Acid Rain	kg SO ₂	0.78	0.10	0.22	10'0	0.00	0.04	0.04	0.29	0.00	0.00	0.00	0.06
Precursors	Equiv.					_					-		
	%	100	13.35	28.51	1.29	0.42	4.87	5.44	37.79	0.51	0.24	0.00	7.26
Ground Level	kg NOX	0.93	0.08	0.32	0.01	10.0	0.06	0.08	0.06	0.02	0.00	0.15	0.15
Ozone	+ 200												
	%	100	8.29	34.34	1.08	09.0	5.99	8.16	6.01	1.92	0.34	16.68	15.63

Table 6.18: Marginal Sensitivity of Input to Product Ratio for Significant Unit Processes in the E85-Corn System (1% increase in input required to produce same product)

	1%1)	increase	(1 % increase in input required to produce same proc	equired to	o produce	e same pr	ō
Stressor	Units	Bascline	Units Baseline Produce Produce Refinery Operate	Produce	Refinery	Operate	
			Com	Ethanol		Vehicle	
Greenhouse kg CO2	kg CO2	224.66	% 10.0	0.29 %	0.29 % 0.10 %	0.77 %	
Gases	Equiv.						
Acid Rain	kg SO2	0.78	0.78 0.01 % 0.44 % 0.38 % 0.93 %	0.44 %	0.38 %	0.93 %	
Precursors	Equiv						
Ground Level kg NOx	kg NOX	6.03	0.02 %	0.45 %	0.45 % 0.06 %	0.84 %	
Ozone	+ VOC					·	

	(1%	increase	e in envi	(1% increase in environmental outputs to produce same product)	l output	ts to pro	oduce san	ne prodı	ict)					
Stressor	Units	Units Baseline Produce		Transport	Produce	Com	Transport	Produce	Transport	Produce	Refinery	Transport	Refuel	Operate
			Natural	Natural Gas Corn Storage Corn Ethanol Ethanol Crude Oil Fuel Vehicle Vehicle	Com	Storage	Com	Ethanol	Ethanol	Crude Oil		Fuel	Vehicle	Vchicle
			Gas											
Greenhouse kg CO2 224.66 0.04 %	kg CO2	224.66	0.04 %		0.01 %	0.04 %	0.20 % 0.01 % 0.04 % 0.01 % 0.31 % 0.03 % 0.10 % 0.03 % 0.00 % 0.00 % 0.23 %	0.31 %	0.03 %	0.10%	0.03 %	0.00 %	0.00 %	0.23 %
Gases	Equiv.													
Acid Rain	kg SO2		0.78 0.13 %		0.01 %	0.00 %	0.29 % 0.01 % 0.00 % 0.00 % 0.05 % 0.05 % 0.38 % 0.01 % 0.00 % 0.00 % 0.07 %	0.05 %	0.05 %	0.38 %	0.01 %	0.00 %	0.00 %	0.07 %
Precursors	Equiv													
Ground Level kg NOx	kg NOx		0.93 0.08 %		0.02 %	0.00 %	0.34 % 0.02 % 0.00 % 0.01 % 0.06 % 0.08 % 0.06 % 0.02 % 0.00 % 0.17 % 0.16 %	0.06 %	0.08 %	0.06 %	0.02 %	0.00 %	0.17 %	0.16%
Ozone	+ VOC							•						_

 Table 6.19:
 Marginal Sensitivity of Environmental Outputs to Product Ratio for Each Unit Process in the E85-Corn System

Table 6.20: Identification of Unit Process Data Points with Significant (>0.25%) Sensitivity in the E85-Corn System

		0
Unit Process	Sensitivity of Input Data to	Sensitivity of
	Stressor Categories	Environmental Output
		Data to Stressor Categories
Operate Vehicle	Fuel requirements:	Not sensitive.
	- ARP (0.93)	
	- GLO (0.84)	
	- GHG (0.77)	
Produce Ethanol	Natural gas requirements:	- GHG (0.31)
	- GLO (0.45)	
-	- ARP (0.44)	
	- GHG (0.29)	
Refinery	Crude oil requirements:	Not sensitive.
	- ARP (0.38)	
Produce Crude Oil	Inputs to crude oil production	- ARP (0.38)
	outside system boundary.	
Transport Natural Gas	Not sensitive.	- GLO (0.34)
-		- ARP (0.29)

E85 – Poplar

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r System	
Mean Results of E85-Poplar System	
Results o	
Table 6.21:	

Stressor	Units	Total	Produce	Transport	Produce	Transport		Refinery	Transport	Refuel	Operate
Category			Poplar	Poplar	Ethanol	Ethanol	Crude Oil		Fuel	Vehicle	Vehicle
Greenhouse Gases	kg CO2 Equiv.	-102.71	16.55	3.08	-206.14	3.26	<u> </u>	16.2	0.65	0;0	51.28
Acid Rain Precursors	kg SO2 Equiv.	-0.19	0.14	10'0	-0.70	10.0	0.29	0.00	0.00	0.00	90.0
	•										
Ground	kg NOx	0.48	0.21	10.0	-0.14	0.02	0.06	0.02	0.00	0.15	0.15
Level Ozone											

Table 6.22: Marginal Sensitivity of Input to Product Ratio for Significant Unit Processes in the E85-Poplar System (10/2 increase in innut routired to produce some product)

	(1 % INC	rease in li	(1 % Increase in input required to produce same product)	ed to produ	ice same j	product)
Stressor	Units	Baseline	Produce	Produce Refinery		Operate
			Poplar	Ethanol		Vchicle
Greenhouse kg CO2	kg CO2	-102.71	-0.16%	-0.19%	-0.19 % -0.22 %	1.50 %
Gases	Equiv.					
Acid Rain	kg SO2	-0.19	-0.74 %		-0.78 % -1.55 %	1.30 %
Precursors	Equiv					
Ground Level kg NOx +	kg NOx +	0.48	0.44 %	0.47 %	0.47 % 0.12 %	0.70 %
Ozone	voc					

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	Syster	n (1% in	icrease i	n environ	mental c	System (1% increase in environmental outputs or reductions to produce same product)	reduction	is to prod	uce same	product	(1
	Units	Baseline	Produce	Transport	Produce	3ascline Produce Transport Produce Transport Produce Refinery Transport Refuel Operate	Produce	Refinery	Transport	Refuel	Operate
			Poplar	Biomass	Ethanol	Ethanol	Crude Oil	,	Fuel	Vehicle	Vchicle
	kg CO2	-102.71	-0.16 %	-0.03 %	2.01 %	-0.03 %	-0.22 %	-0.06 %	-0.01 %	0.00 %	-0.50 %
	Equiv.										
	kg SO2	-0.19	-0.74 %	-0.04 %	3.71 %	-0.05 %	-1.55 %	-0.02 %	-0.01 %	0.00 %	-0.19 -0.74 % -0.04 % 3.71 % -0.05 % -1.55 % -0.02 % -0.01 % 0.00 % -0.30 %
	Equiv										<u> </u>
	Ground Level kg GLO	0.48	0.44 %	0.03 %	-0.28 %	0.03 %	0.12 %	0.04 %	0.01 %	0.32 %	.48 0.44 % 0.03 % -0.28 % 0.03 % 0.12 % 0.04 % 0.01 % 0.32 % 0.30 %
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: E85-Poplar System	
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Table 6.24:	I'mit Proces Cencitivity

Unit Process	Sensitivity of Input Data to	Sensitivity of
	Stressor Categories	Environmental Output
		Data to Stressor Categories
Operate Vehicle	Fuel requirements:	- GIIG (-0.50)
	- ARP (1.30)	- ARP (-0.30)
	- GLO (0.70)	- GLO (0.30)
	- GHG (1.50)	
Produce Ethanol	Poplar requirements:	- GHG (2.01)
	- GLO (0.47)	- ARP (3.71)
	- ARP (-0.78)	- GLO (-0.28)
Produce Poplar	Land area requirements:	- ARP (-0.74)
	- ARP (-0.74)	- GLO (0.44)
	- GLO (0.44)	
Refinery	Crude oil requirements:	Not sensitive.
	- ARP (-1.55)	
Produce Crude Oil	Inputs to crude oil production	- ARP (-1.55)
	outside system boundary.	
Refuel Vehicle	Not sensitive.	- GLO (0.32)
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Marginal sensitivity analysis has identified all the unit processes with the greatest sensitivity on the overall results for each fuel system. Given the public data resources available for completing this LCA, each sensitive unit process is currently using the best known available data values.

6.3.4 Results and Uncertainty Analysis

This LCA considered three sources of uncertainty: uncertainty in the ratio of inputs to products for each unit process, uncertainty in the ratio of environmental outputs to products for each unit process, and uncertainty in the environmental outputs not accounted for upstream of the selected system boundary. Modeling of the first two data uncertainties is completed using Monte Carlo Analysis (Figure 6.1 – Step 5) [17]. Uncertainty associated with system boundary selection is analyzed using the results from the RMEE method (Figure 6.1 - Step 2) [19].

Uncertainty Due to System Data

For any analysis, a degree of uncertainty is associated with each input and each emission of each unit process. Uncertainty in each data point is either provided by the data source, or it is assumed to be \pm . Monte Carlo Analysis is then run with 2000 iterations applying normally distributed random values for each data point. Statistical analysis on the 2000 iterations provides a mean (X_{Zj}) and standard deviation for the system results, which allows one to calculate the 95% confidence interval for the results (r_{data}) [19].

Uncertainty Due to System Boundary Selection

The RMEE method results in an adjustment factor (Y_{ZMean}) ranging from 0 to 100, which is applied to the mean results generated by the Monte Carlo Analysis of the data for each system (X_{Zj}) . The RMEE adjustment factor has a probability distribution, which is a skewed non-normal as defined by *Raynolds et al* [17]. The distribution of Y_{ZMean} is modeled as a truncated-normal distribution [17].

Combining Data and System Boundary Uncertainty

To calculate the overall mean results (X_{Z_j}) and 95% confidence interval (r_{Total}) , the results from the system data (X_{Z_j}) are adjusted to account for the system boundary using equation 3.2 from Raynolds et al [17] (repeated here for clarity).

$$X_{zj}^{'} = \frac{X_{zj}}{Y_{zMean} / 100}$$
(3.2)

Because both Y_{ZMean} and X_{Zj} have an uncertainty associated with them and the distribution of Y_{ZMean} is non-normal, the most practical method to calculate the overall uncertainty is through the use of Monte Carlo Analysis (Figure 6.1 – Step 5) [17]. Monte Carlo Analysis is applied to equation 3.2, as demonstrated by Raynolds et al [17], to produce a distribution for X_{Zj} . This is completed for each stressor category and for each system. Using the distribution, the 95% confidence interval for each system can be calculated by taking 2.5% off of each tail of the distribution. The adjusted mean and 95% confidence interval for each system and each stressor category are presented in Figures 6.6 through 6.8.



Figure 6.6: Mean and Uncertainty (95% Confidence) of Greenhouse Gas Emissions



Figure 6.7: Mean and Uncertainty (95% Confidence) of Acid Rain Precursor Emissions



Figure 6.8: Mean and Uncertainty (95% Confidence) of Ground Level Ozone Precursor Emissions

6.3.5 Discussion of Results – Do the Results Allow for a Decision?

As illustrated in Figures 6.6, 6.7, and 6.8 above, the results show significant overlap in uncertainties of a number of systems. However, depending on the specific decision to be made, the results do allow for decision making. For example, if the decision is to select the fuel with the least potential greenhouse gases (GHG), it is clear the E85-Poplar system is the best choice. Its 95% confidence interval is clearly distanced from all other three options. However, for ARP and GLO the uncertainty of the E85-Poplar system does overlap with other systems.

The decision maker should be aware of the level of confidence to have in the relative comparison for each stressor category. To calculate this confidence, the distributions resulting from the Monte Carlo Analysis used to combine data uncertainty with system boundary uncertainty are used to calculate the probability the stressor category of one system is less than another (Figure 6.1 – Step 7) [17]. The results of calculating the confidence that one system will result in less emissions of each stressor category than another system are presented in Table 6.25. The results indicate a high level of confidence (above 80%) that both ethanol systems (E85-Corn and E85-Poplar) result in lower emissions of greenhouse gases (GHG). There is also a high level of confidence (98.1%) that E85-Poplar results in the least acid rain precursors (ARP). However, with respect to ground level ozone (GLO), the confidence that E85-Poplar results in fewer emissions is low (45.2%). The GLO emissions of the E85-Poplar system are more likely (54.8%) to be equal to the emissions of the next lowest emitter of GLO – the RFG system.

If a decision was to be made based on ground level ozone potential, the low confidence in the relative performance of the E85-Poplar system for GLO emissions might prevent the decision maker from deciding to promote E85-Poplar (Figure 6.1 -Step 8). If the confidence level was higher (above 75%), the decision maker would most likely proceed to the Impact Analysis stage of LCA and draw final conclusions and recommendations. If the confidence level of all three stressor categories were significantly low, there would

be no question but to proceed to Uncertainty Reduction Analysis (Figure 6.1 – Step 9). Because the E85-Poplar system clearly results in less GHG and ARP emissions, (although there is low confidence that the system results in fewer GLO emissions), the decision maker may wish to proceed to Impact Analysis to consider the relative significance of each stressor category.

For the purpose of this paper, it is assumed the decision maker has proceeded to the Impact Analysis, but still considers it valuable to determine how the uncertainty can be reduced. As a result, the next step in the Inventory Assessment is to complete an Uncertainty Reduction Analysis (Figure 6.1 -Step 9) [17].

Table 6.25:	Probability the Mean of System i is Less than the Mean of System j
	for Each Stressor Category

Stressor Category	System i	System j	Probability i <j< th=""></j<>	
GHG	CNG	RFG	55.6%	
	E85-Corn	CNG	83.3%	
	E85-Poplar	E85-Com	100%	
ARP	E85-Corn	RFG	70.4%	
	CNG	E85-Corn	29.1%	
	E85-Poplar	CNG	98.1%	
GLO	CNG	E85-Corn	40.5%	
	RFG	CNG	63.6%	
	E85-Poplar	RFG	45.2%	

Investigation of the Contributions to Overall Uncertainty – Uncertainty Reduction Analysis

Raynolds et al [19] developed a technique to evaluate the potential reduction in overall uncertainty by systematically removing the uncertainty in individual unit process data. This has been applied to the most sensitive unit processes identified above in Tables 6.12, 16, 20 and 24 for each system (Figure 6.1 – Step 9). The potential reduction in uncertainty as a result of expanding the system boundary to $Z_{RMEE} = 0.10$ has also been evaluated. The results for the four fuel systems are illustrated in Figures 6.9, 6.10, 6.11, and 6.12. As shown by the results, the single largest opportunity for reducing uncertainty in the GHG results of each system is to expand the system boundary to $Z_{RMEE} = 0.10$. By expanding the system boundary, the total uncertainty in each system can be reduced by at least 25%. The potential for reducing total uncertainty in GHG emissions through improving data sets is limited. As a result, if time and resources are made available to reduce uncertainty in the GHG results, it is most effective to expand the system boundary. Investing time and resources in reducing GHG uncertainty would only be appropriate if a decision had to be made between the RFG and the CNG system because as shown in Table 6.25, this is the only decision with a relatively low confidence (55.6%).

When comparing the options for reducing uncertainty in the results of ARP, each system has different unit processes where improved data quality would have a significant impact on uncertainty. For the RFG, E85-Corn, and E85-Poplar systems, improved data on the "Produce Crude Oil" unit process will have the most significant impact on reducing overall uncertainty in ARP emissions. For the CNG system, the unit process to focus on is "Operate Vehicle". Investing time and resources in improving these data sets would only make sense if one was deciding between RFG, CNG and E85-Corn, since it is clear the E85-Poplar system results in the fewest ARP emissions.

For ground level ozone (GLO) emissions, a mix of strategies exist for reducing uncertainty and increasing the confidence in the decision. As shown in Figure 6.9, the most effective means to reduce uncertainty in the RFG system is to reduce the uncertainty in the "Produce Crude Oil" unit process. For the CNG system, time and resources allocated to reducing the uncertainty in the "Operate Vehicle" unit process will be most effective (Figure 6.1 – Step 11). To reduce the uncertainty of GLO emissions for the two ethanol system, the greatest potential lies in expanding the system boundary (Figure 6.1 – Step 12). In attempting to obtain data to reduce the uncertainty in unit processes and expand the system boundary, it was discovered very few data sets are currently available. As a result, the decision has been made (Figure 6.1 -Step 10) to proceed to Impact Analysis and not reiterate the Inventory Assessment.

6.3.6 Impact Analysis

Having completed the Inventory Assessment through the collection of tools developed by *Raynolds et al* [17][18][19], the next step in LCA is to complete the Impact Analysis. Because the primary purpose of this LCA is to demonstrate the uncertainty and system boundary techniques illustrated in Figure 6.1, this analysis does not complete an Impact Analysis to investigate the environmental significance of each environmental stressor category. Nevertheless, the results clearly show, that on a relative basis, the E85-Poplar system results in the least potential for contributing to climate change through the emissions of greenhouse gases, and the least potential for contributing to acid rain. However, there is a lower confidence in the E85-Poplar system's relative performance on ground level ozone precursors so it is unclear whether E85-Poplar would give significant smog reduction as compared to the other options.



Figure 6.9: The potential reduction in overall uncertainty of the RFG System by eliminating uncertainty in the most sensitive unit processes and by expanding the system boundary to $Z_{RMEE}=0.10$



Figure 6.10: The potential reduction in overall uncertainty of the CNG System by eliminating uncertainty in the most sensitive unit processes and by expanding the system boundary to $Z_{RMEE}=0.10$



Figure 6.11: The potential reduction in overall uncertainty of the E85-Corn System by eliminating uncertainty in the most sensitive unit processes and by expanding the system boundary to Z_{RMEE} =0.10



Figure 6.12: The potential reduction in overall uncertainty of the E85-Poplar System by eliminating uncertainty in the most sensitive unit processes and by expanding the system boundary to $Z_{RMEE} = 0.10$

6.4 Conclusions

- With almost 100% confidence it can be concluded that an 85% ethanol blend fuel derived from poplar will result in less greenhouse gas emissions than reformulated gasoline, compressed natural gas, and ethanol blends derived from corn.
- With over 98% confidence it can be concluded the E85-Poplar system will result in less emissions of acid rain precursors than the other fuels analyzed.
- Due to uncertainty in ground level ozone emissions it is difficult to conclude with confidence whether or not the E85-Poplar system results in less smog precursor emissions. This uncertainty can be best reduced by expanding the system boundary to Z_{RMEE} =0.10 and reducing the uncertainty in the "Produce Crude Oil" unit process.
- The collection of tools for quantifying data uncertainty, system boundary uncertainty and total uncertainty, and for identifying the most effective allocation of time and resources to reducing the total uncertainty is a practical method for guiding the LCA practitioner through the inventory assessment stage of LCA. It has been demonstrated that the use of these tools collectively allows the LCA practitioner to provide recommendations to the decision maker with known confidence.

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Chapter 7

Conclusions

Chapter 7 – Conclusions

By investigating the current practices of completing the life-cycle inventory (LCI) phase of life-cycle assessment (LCA), it has been shown that a need exists to provide rigorous and quantitative tools for selecting system boundaries and assessing uncertainty. This need will only be increased as emission trading systems develop and will require accurate and repeatable quantification of emission reductions. In response to this need, this research has resulted in the design, development and testing of the following tools for use in the LCI stage of LCA:

- 1. Relative Mass-Energy-Economic (RMEE) for System Boundary Selection provides a repeatable quantitative method for selecting comparable system boundaries for competing systems and provides an estimate of the contribution of uncertainty in overall results due to system boundary selection. The RMEE method has been designed and tested for comparing energy and product systems based on common combustion-related air emissions. System boundaries are defined by Z_{RMEE} representing the ratio of the mass, energy or economic value of any given input of the system to the functional unit of the LCA. The basic assumption under which RMEE is effective is that the mass, energy or economic value of environmental outputs being evaluated. As a result, evaluation of toxic releases or other small but important environmental outputs with RMEE is only possible if the externality costs of these releases are captured in the value of the product.
- 2. Marginal Sensitivity Analysis provides a systematic method of testing the sensitivity of each data point in a system on the overall results. This tool is effective in identifying sensitive data points early in the LCI. It systematically increases the environmental outputs and material input requirements by 1% for a given product of a unit process. The results show the marginal change in the total system and quickly highlight the most sensitive data points.
- 3. Monte Carlo Analysis for Calculating Error Propagation in LCA Data provides a numerical method for calculating the overall uncertainty in a system due to uncertainty in data. By utilizing the Monte Carlo technique of randomly

selecting data points from a defined distribution and iterating this over 1000 times, the propagation of error throughout the life-cycle system can be calculated. The result is an error range for each environmental output in the LCI. The advantage of the Monte Carlo Analysis technique is it can combine symmetric and non-symmetric distributions of data.

- 4. Monte Carlo Analysis for Combining Data Uncertainty and System Boundary Uncertainty – provides a numerical method for calculating the overall total uncertainty in the inventory results of an LCA as a result of both uncertainty in data and uncertainty in system boundary selection. Monte Carlo Analysis is applied here because the distribution of uncertainty due to system boundary selection (derived from RMEE) is not normally distributed and the uncertainty from error propagation is also not necessarily symmetrical.
- 5. Calculation of Confidence in Relative Performance uses the histograms resulting from the Monte Carlo Analysis combining data and system boundary uncertainty to calculate the probability or confidence of one system resulting in lesser output of a given environmental stressor category than a competing system. This tool allows the decision-maker to know the confidence level at which the emissions from System X are less than the emissions from System Y.
- 6. Uncertainty Reduction Analysis provides an efficient method of estimating the potential reduction in overall uncertainty by eliminating uncertainty in the data for specific unit processes. This technique answers the question: "If the uncertainty in Unit Process A was zero, how would this affect the overall uncertainty?". This allows for efficient allocation of time and resources in reducing overall uncertainty in decision making.

Together, these six tools provide a means to advance the LCA field. The package creates a set of rules for LCA professionals to follow when completing LCI. In practice this will lead to more repeatable and defendable results in the Inventory stage of LCA studies. Through the testing of this systematic method, the following conclusions have been made:

- Marginal Sensitivity Analysis is an effective tool for identifying early in the inventory stage the data points having the greatest impact on the overall results.
- The RMEE method relies on a clear correlation between mass, energy or economic value of products and the resulting environmental outputs. As a result, the RMEE technique is recommended for LCA studies of energy and product systems where a comparison of combustion emissions is being made.
 Combustion-related air emissions are assumed to be directly proportional to the mass, energy or economic value of a fuel product. Additional tools and techniques need to be developed to evaluate environmental outputs (e.g. toxic releases) which may not be correlated to mass, energy or economic value of products.
- When the above conditions are satisfied, the Relative Mass-Energy-Economic (RMEE) of system boundary selection is a rigorous and repeatable method allowing the LCA practitioner to streamline LCA and focus on the unit processes most relevant to the decision.
- The application of RMEE to over 1000 different randomly generated systems has provided a method to estimate the uncertainty in the final results associated with the system boundary selected by a particular Z_{RMEE} cut-off ratio. It has been found that Z_{RMEE} values greater than 0.25 introduce a significant amount of uncertainty to the results. The distribution of the mean fraction of the true total environmental output of a system (Y_{ZMean}) at a given Z_{RMEE} value is found to be non-symmetrical. For the purpose of modeling, this distribution is considered to be normally distributed but truncated at Y_{ZMean} equal to 100%. This has been shown to be appropriate for Z_{RMEE} values less than 0.25.
- The uncertainty associated with system boundary selection is dependent on whether the LCA system is being modeled as a mass conserving system or a nonmass conserving system (e.g. biomass production). The evaluation of random systems for both types has shown that non-mass conserving systems will have

greater uncertainty associated with the system boundary for any given Z_{RMEE} value.

- Monte Carlo Analysis provides a practical method of calculating the propagation of data error throughout a LCA system. The flexibility of Monte Carlo Analysis allows for evaluation of non-normal distributions of error in unit processes.
- Uncertainty Reduction Analysis is an effective tool for identifying where one should consider committing time and resources to reduce the overall uncertainty in the results.
- Monte Carlo Analysis is a practical numerical method for combining the uncertainties associated with data and system boundaries because both of these uncertainties may be non-symmetrically distributed.
- Using the histograms generated from the Monte Carlo Analysis to combine uncertainties, the decision maker can be presented with a confidence level on whether one system results in fewer emissions of an environmental stressor category than a competing system.
- The combination of the six tools described above provides a practical package of tools for streamlining the completion of the Inventory Assessment stage of LCA.
- The application of the six tools to Inventory Assessment provides a repeatable and quantitative method for identifying the most sensitive data values, selecting system boundaries, quantifying overall uncertainty and identifying the most effective opportunities for reducing uncertainty.

The advanced inventory method has been applied to a study of various automotive fuels including MTBE reformulated gasoline, natural gas, and 85% ethanol blends (E85) from two different sources of ethanol (corn and poplar). The results show that E85 from poplar trees should result in the least emissions of greenhouse gases and acid rain precursors with over 95% confidence. The system should also produce less ground level ozone precursors but with only 45% confidence. The LCI tools were shown to be effective in selecting system boundaries and providing the decision-maker with a level of confidence in the LCI.

Appendix I

Case Study – A Life-Cycle Comparison of Ethanol Feedstock Options and Technologies for Canada

Appendix I presents a published paper applying life-cycle assessment to six different sources of ethanol fuel. The RMEE method of system boundary selection is applied.

Appendix I: A Life-Cycle Comparison of Ethanol Feedstock Options and Technologies for Canada

[Published at the "Combustion and Global Climate Change" conference, 1999]

Introduction

Canada is committed to reduce its greenhouse gases over the next decade. With approximately 30% of Canada's greenhouse gas emissions originating from the transportation sector, the country is searching for more carbon-efficient transportation fuels [1]. Bio-fuels can potentially reduce greenhouse gas emissions as they are considered CO₂ "neutral" during combustion [2][3]. However, the raw material extraction and processing energy involved in producing bio-fuels can be significant. An example is ethanol fuel, where significant upstream differences exist between feedstock growth and conversion. To fairly compare fuels with different feedstocks and different production processes, a life-cycle approach of analysis is required.

Life cycle assessment (LCA) has evolved over the past 20 years to become a useful tool for comparing alternative products and services. Although in wide use, the field of LCA has not come to consensus on a number of key methodology issues including system boundary selection and uncertainty analysis. This paper uses an LCA approach to compare three feedstocks for producing ethanol fuel: corn, wheat, and poplar trees. The approach taken focuses on selecting consistent system boundaries for each fuel system and on making a reasonable assessment of uncertainty before conclusions are drawn.

The data sets for this LCA are limited to publicly available sources and they have not been externally reviewed for accuracy. Hence, the reader should take caution in basing decisions on the results presented here. This data set is not sufficiently comprehensive to fully compare the alternative feedstock options for ethanol production. Of particular interest to the LCA practitioner will be the Relative Mass-Energy-Economic (RMEE) method of selecting system boundaries and the demonstration of Monte Carlo analysis for assessing uncertainty in results. Ethanol producers will be shown the results of applying publicly available data to a life cycle analysis of ethanol production.

This paper is organized by the general steps of Life Cycle Assessment – goal definition, scoping, inventory assessment, and impact analysis.

Goal Definition

Objective

The objective of this life-cycle assessment (LCA) is to utilize publicly available data to compare the lifecycle environmental performance of producing fuel ethanol from three Canadian feedstocks: corn, wheat and poplar trees. This LCA also compares four different technologies for converting the poplar trees to ethanol: three different strong acid scenarios and an enzymatic process.

Systems or Feedstock Options for Ethanol Production

There are numerous feedstock options for producing ethanol including corn, wheat, poplar trees, grasses, sugar cane, artichokes, waste biomass, and potentially most other forms of biomass. This work has chosen three feedstocks to consider: corn, wheat and poplar trees. The first two are commonly used ethanol feedstocks and are both in use by ethanol plants currently operating in Canada. The third, poplar trees, is recognized to be a potentially viable ethanol feedstock using new technology for converting lignocellulose feedstocks to ethanol [4] [5]. Table 1 summarizes the ethanol feedstock options considered by this study.

A range of technologies exists for converting each feedstock. Conversion technologies for corn and wheat have long existed and are well established. For this work, publicly available data from operating ethanol plants in Canada were used to assess the corn and wheat feedstock options. Technology to convert poplar trees to ethanol has existed since the Second World War [6], but could not compete economically with conventional fuels or grain ethanol. Technologies have been developed over the past decade to convert lignocellulose feedstock to ethanol, including various enzymatic processes and acid processes [5]. This study utilizes publicly available data sets covering the input and output requirements for two different strong acid conversion processes and one enzymatic process. Three poplar tree options utilize co-generation to provide steam and power, while the wheat, corn and one poplar tree option do not. The six system configurations compared by this analysis are described in Table 2.

Table 1: Ethanol Feedstock Options Considered

Feedstock	Reason for Inclusion
corn	The majority (over 80 %) of ethanol currently produced in Canada is from corn [4].
wheat	Wheat is the primary feedstock for ethanol production in Western Canada [4].
poplar trees	Poplar trees are potentially one of the most economically feasible biomass feedstocks in Western Canada[4].

	System	Description
1	Corn Without	Corn ethanol system operating in Southern Ontario without on-site electricity
	Cogeneration	cogeneration. Required electric power is provided by the average Ontario
		grid.
2	Wheat Without	Wheat ethanol system operating in the Prairies without on-site cogeneration.
	Cogeneration	Power is assumed to be provided by the average Alberta grid.
3	Poplar Strong Acid	Poplar tree ethanol system operating in Alberta utilizing a strong acid
•	Without	conversion technology [6] without cogeneration. Power is provided by the
	Cogeneration	average Alberta grid.
4	Poplar Strong Acid	Poplar tree ethanol system operating in Alberta utilizing a strong acid
1.	System (I) With	conversion technology [6] with on-site cogeneration to provide steam
	Cogeneration	requirements and sell excess power. For every 1000 liters of ethanol
		produced, 348 kWh of excess electricity are produced. Additional power
		requirements provided by average Alberta grid.
5	Poplar Strong Acid	Poplar tree ethanol system operating in Alberta utilizing a strong acid
•	System (II) With	conversion technology [7] with on-site cogeneration to provide steam
	Cogeneration	requirements and sell excess power. This configuration of cogeneration has
		the highest power-to-ethanol ratio (3592kWh per 1000 liters ethanol
		produced). It is used to define the functional unit of 1000 liters of ethanol
		and 3592 kWh of electricity.
6	Poplar Enzymatic	Poplar tree ethanol system operating in Alberta utilizing an enzymatic
	System With	conversion technology [7] with on-site cogeneration to provide steam
	Cogeneration	requirements and sell excess power. For every 1000 liters of ethanol
		produced, 1886 kWh of excess electricity are produced. Additional power
		requirements provided by average Alberta grid.

Table 2: Six Ethanol Production Systems Analyzed

Audience

Decision makers and LCA practitioners will be interested in the demonstration of the RMEE method for system boundary selection and the use of Monte Carlo analysis for uncertainty analysis. The ethanol industry and government policy makers will take interest in the results and conclusions of the LCA study based on publicly available data.

Limitations and Boundaries

This LCA:

• does not include an analysis of life-cycle economics,

- is limited to public data sources, some of which have not been externally peer reviewed,
- is "cradle-to-fuel", i.e. does not include the use of the fuel since the fuels are identical,
- considers only Canadian feedstock scenarios,
- does not compare ethanol to an accepted base case such as gasoline,
- does not consider detailed system design improvements,
- does not consider the geographical relevance of environmental outputs.

Scoping

Functional Unit

The functional unit for this LCA has been selected as 1000 liters of fuel grade ethanol and 3592 kWh of electricity. This ratio of fuel production to electricity generation is chosen based on the largest ratio from the three co-generation systems analyzed – Poplar Strong Acid System (II) With Cogeneration.

Environmental Stressor Categories

Table 3 presents the three environmental stressor categories selected for analysis by this LCA. All three stressors are key anthropogenic atmospheric pollution problems. Since much of the interest in biofuels arises from greenhouse gas emissions, it is reasonable to concentrate on differences in air pollutant emissions for the systems being considered. However, it is worth noting the lack of available data on water effluents (e.g.Biological Oxygen Demand) and other waste streams. The three stressor categories (greenhouse gases, acid rain precursors, and ground level ozone precursors) provide an indication of the relevant environmental performance of different technologies. The contributing factors to each stressor category are shown in Table 4. Each stressor category has two or more contributing pollutants each with a weighting factor to report the results in "equivalents".

Stressor Category	Discussion		
1. Greenhouse Gases	Potential impact is climate change through enhanced greenhouse effect. Canada has agreed to reduce emissions to 6% below 1990 levels through the United Nations Framework Convention on Climate Change.		
2. Acid Rain Precursors	Acid forming emissions lead to regional acid deposition with potential impacts on flora and fauna due to lowered pH in soils and water.		
3. Ground Level Ozone Precursors	Ground level ozone, known commonly as smog, is considered to have a negative impact on human health (respiratory problems) and plant growth.		

Table 3: Selected Environmental Stressor Categories

Stressor Category	Stressor Category Units	Contributing Factors	Weighting of Factor [8]
Greenhouse Gases	kg CO ₂ Equivalent	CO ₂ CH ₄ N ₂ O	1 21 320
Acid Rain Precursors	kg SO ₂ Equivalents	SO ₂ NOx	1 0.70
Ground Level Ozone	kg (VOC + NOx)	VOCs NOx	1 1

Process Flow Diagrams

Figures 1 through 6 illustrate the ethanol fuel production systems considered by this LCVA. The full box shows all the processes initially considered and the smaller grey area identifies the system boundary finally used in the study for each system. Setting this boundary in a logical and repeatable manner is the purpose of the Relative Mass-Energy-Economic (RMEE) method, discussed in more detail below.

Figure 1: Corn System With No Cogeneration







Figure 3: Poplar Strong Acid System with No Cogeneration



Figure 4: Poplar Strong Acid System (I) With Cogeneration











Inventory Assessment

System Boundary Selection

<u>"Cradle-to-fuel"</u> As shown in Figures 1 through 6, this study considers only the unit processes from "cradle-to-fuel". The use phase of the ethanol fuel is not considered. The reasoning behind this is that each system produces an identical product – fuel ethanol and electricity. The purpose of this LCA is to differentiate between ethanol production using different feedstocks and processes so the emissions from downstream combustion (equal for all six systems) have been excluded from this work.

<u>Geography</u> Ethanol feedstocks and production facilities are assumed to be located in Canada. As a result, all feedstock production data reflect the yields expected in the Canadian climate.

<u>Time and Technology</u> This LCA takes a "snap-shot" in time (data from 1994 through 1998, see Tables 6, 7, 8 and 9) utilizing the most currently available data for each unit process. No attempt has been made to consider changes in performance as technology evolves over time. The technology used for ethanol

conversion for corn and wheat is the current technology in operation in Canada [9]. For the poplar systems, two different strong acid technologies and one enzymatic technology for converting poplar to ethanol are evaluated. With respect to the source of electricity, the provincial grid average is applied (Ontario grid for corn ethanol, Alberta grid for all other systems).

Boundary Selection: Unit Process Cut-Off with the RMEE Method The Relative Mass-Energy-Economic (RMEE - pronounced 'army') method for system boundary selection has been used to select the system boundary [10]. One of the critical problems in any LCA is to decide which inputs need to be followed and which can reasonably be ignored, thus setting the "boundaries" of the analysis. At each unit process, the RMEE method calculates the ratio of each input to the functional unit on a mass basis, energy basis and economic basis. If any of these three ratios is greater than a chosen cut-off ratio that input is included in the system boundaries. The RMEE method has been more completely described in [10].

The RMEE system boundary cut-off ratio selected for this LCA was 0.15 meaning if the mass, energy or market value of any input to a unit process is greater than 15% of the mass, energy or market value of the functional unit then the upstream unit processes are considered inside the system boundary. Due to limited data availability, a 0.15 cut-off was the lowest value feasible with the time and resources available for this LCA. A 0.15 cut-off ratio is appropriate for producing preliminary results, but as shown in the process flow diagrams (Figures 1 through 6), it can cut a great deal of detail out of the system.

Allocation Method

Another critical area in any LCA is the allocation of unit process inputs and environmental outputs between the main product and the co-products that are simultaneously produced. This LCA did not attempt to expand system boundaries of each ethanol production system to include the use and equivalence of all coproducts. Instead, allocation of environmental outputs and unit process inputs to products is completed by market value allocation. The only unit process in each system, which produces multiple products, is the ethanol conversion plant. The allocation of inputs and environmental outputs to each product of each ethanol plant is shown in Table 5. Plant emissions are NOT allocated to the production of electricity from cogeneration, since the electricity is defined as part of the functional unit. Therefore, the ethanol plant emissions associated with electricity production are already accounted for by ensuring each of the systems provides similar amounts of electricity. It is assumed that electricity produced from the cogeneration systems directly off-sets electricity from the grid.

As Table 5 shows, the poplar systems allocate a significantly larger fraction (81.1% opposed to 50-60%) of the upstream inputs and emissions to the ethanol fuel compared with the corn and wheat systems. The main co-product of the poplar system is lignin, which is assumed to be combusted on-site to provide energy for steam production. This use of lignin directly off-sets the use of natural gas and therefore indirectly allocates the lignin co-product equivalent to natural gas on an energy basis.

Table 5: Allocation to Ethanol Conversion Products

				System			
Product	Corn w/o Cogen. (%)	Wheat w/o Cogen. (%)	Poplar Strong Acid w/o Cogen. (%)	Poplar Strong Acid (I) w/ Cogen. (%)	Poplar Strong Acid (II) w/ Cogen. (%)	Poplar Enzymatic w/ Cogen. (%)	Assumed Market Value
Ethanol	54.5	58.3	81.1	81.1	81.1	81.1	0.30 S/liter
Distillers Dried Grains and Solubles (DDGS)	33.8	41.7	n/a	n/a	n/a	n/a	0.22 \$/kg [11]
Captured Carbon Dioxide	11.7	0 (not capture d)	18.7	18.7	18.7	18.7	0.10 S/kg [12]
Lignin	n/a	n/a	0 (combusted as fuel)	0 (combusted as fuel)	0 (combusted as fuel)	0 (combusted as fuel)	n/a
Gypsum	n/a	n/a	0.01	0.01	0.01	0.01	0.008 \$/kg [6]

n/a = not applicable i.e. not produced by the system
¹ Market value of ethanol assumed to be equal to the market value of MTBE, the oxygenate most likely to be replaced by ethanol.

Data Sources and Uncertainty

Tables 6 through 9 present the data sources and assumptions made for each unit process in each of the three systems.

Unit Process	Data Sources	Assumptions
Corn Ethanol Conversion	Commercial Alcohols (1995) [9]	• Emission factors from natural gas combustion in "industrial size boiler" – AP-42 [13]
Supply Water	City of Chattam (1998)	• Emission factors from natural gas combustion in "industrial size boiler" - AP-42 [13]
Transport Corn	Deluchi [2], Mobile 5a	Corn transported 60 km.
Corn Storage and Handling	Agriculture and Agri- Food Canada (1996) [14]	• Emissions from combustion of propane for drying.
Corn Harvest	Agriculture and Agri- Food Canada (1996) [14]	 Mean harvest is 6,660kg per hectare.
Corn Farm	Agriculture and Agri- Food Canada (1996) [14]	 Electricity consumption based on average use of electricity in Canada for agriculture. Moldboard plow for tillage.

Table 6: Data Sources and Assumptions for the Corn System

Table 7: Data Sources and Assur	mptions for the Wheat System
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Unit Process	Data Sources	Assumptions
Wheat Ethanol Conversion	Pound Maker ethanol plant, Lanigan Saskatchewan (1994, 1998) [15]	• Emission factors from natural gas combustion in "industrial size boiler" - AP-42 [13]
Supply Water	Lanigan Ethanol Plant	• Water for ethanol plant from natural sources.
Transport Wheat	Deluchi [2], Mobile 5a	Wheat transported 60 km.
Wheat Harvest	Agriculture and Agri-Food Canada [16]	• Mean harvest is 1,559 kg per hectare.
Wheat Farm	Coxworth [17] (1994)	 Diesel emissions from tractor. Electricity consumption based on average use of electricity in Canada for agriculture.
Transport Crop Protectants	Deluchi [2], Mobile 5a	Transported 1000 km.
Produce Crop Protectants	M. Wang, Argonne National Lab (1998) [3]	• Emissions based on fuel combustion from AP-42 emission factors.

Table 8: Data Sources and Assumptions for the Poplar Systems

Unit Process	Data Sources	Assumptions
Poplar Ethanol Conversion Plant - Strong Acid (I) Without Cogeneration Poplar Ethanol Conversion Plant - Strong Acid (I) With Cogeneration	Arkenol (1998) [6] Arkenol (1998) [6]	 Hypothetical plant for general biomass source located in rural Alberta. Lignin co-product is combusted to produce steam. Conventional boiler (85% efficiency) Zero CO2 emissions from lignin combustion. Supplemental fuel for steam is natural gas. Emission factors from natural gas combustion in "industrial size boiler" - AP-42 [13] As above except conventional boiler replaced with cogeneration: Cogeneration system based on optimizing system for process steam requirements.
Poplar Ethanol Conversion Plant – Strong Acid (II) With Cogeneration Poplar Ethanol Conversion Plant – Enzymatic With Cogeneration	NREL (1998) [7] NREL (1998) [7]	 Strong acid technology similar to Arkenol Inc. technology but modeled by NREL using a simulation software. Emission factors from natural gas combustion in "industrial size boiler" - AP-42 [13] Input and output information developed by NREL using Aspen®-based model. Emission factors from natural gas combustion in "industrial size boiler" - AP-42 [13]
Supply Water	Municipality of Drayton Valley, AB(1998)	• Emission factors from natural gas combustion in "industrial size boiler" – AP-42 [13]
Transport Biomass	Deluchi [2], Mobile 5a	Corn transported 60km.
Poplar Harvest	Farmers and foresters in Drayton Valley, AB region (1998)	• Mean harvest is 6,854 kg per hectare.
Poplar Plantation	Oak Ridge National Laboratory (1997), Agriculture Canada	 Plantation on a 7 year rotation. Diesel emissions from combustion in a tractor. Electricity consumption based on average use of electricity in Canada for agriculture.

Unit Process	Data Sources	Assumptions			
Produce Electricity	Ontario Hydro (1997), TransAlta Utilities (1996)	 Corn system utilizes data from Ontario Hydro, wheat and poplar systems utilize data from TransAlta. Annual average grid emissions are used. 			
Transport Fertilizers	Deluchi [2], Mobile 5a	Transported 1000 km.			
Produce K2O Fertilizer	M. Wang, Argonne National Lab (1998)	• Emissions based on fuel combustion from AP-42 emission factors. [13]			
Produce P2O5 Fertilizer	M. Wang, Argonne National Lab (1998)	• Emissions based on fuel combustion from AP-42 emission factors. [13]			
Produce N Fertilizer	M. Wang, Argonne National Lab (1998)	• Emissions based on fuel combustion from AP-42 emission factors. [13]			
Upstream Natural Gas	Monenco (1992) [18]	• Includes emissions from exploratory drilling, development drilling, processing, pipeline transport, and flaring.			

Table 9: Data Sources and Assumptions Common to all Systems

Modeling

Modeling of each system was completed using an LCA software model developed by the principal author. The software model accumulated data on unit processes and the links between them, evaluated equivalent cut-off boundaries using the RMEE method, then calculated the overall inputs and stressor outputs for each system. A Monte Carlo random input technique was used to estimate overall uncertainty of the analysis and to attribute that uncertainty to specific unit processes.

Monte Carlo Analysis

For any analysis, a degree of uncertainty is associated with each input and each emission of each unit process. Due to the lack of statistical data for each unit process, this LCA assumes a conservative 50% uncertainty for each material, service or energy input to each unit process. Likewise, each environmental output is assumed to have a 50% uncertainty. The Monte Carlo technique consists of analyzing the system repeatedly using random, normally distributed input values for each uncertain variable. This study was based on 2000 iterations. Statistical analysis of the results allows the user to measure the uncertainty of a complex system and to identify the unit processes, which contribute the greatest amount of that uncertainty. Future research can then concentrate on improving the data for unit processes with the largest contribution of uncertainty.

System Boundary Selection Adjustments

Using the RMEE method of system boundary selection, the results were adjusted to incorporate the uncertainty introduced by the system boundary [19]. At the system boundary cut-off ratio equal to 0.15, a factor of 1.08 is applied to the inventory results to adjust for the unit processes outside the system boundaries. This factor is based on the results presented in [17] for biomass systems where a large number of random LCA systems were evaluated to obtain a relationship between the system boundary cut-off and uncertainty in results. In addition, random variability in the unit processes, which form the system boundary, introduces a source of uncertainty which, for a cut-off ratio of 0.15, has been estimated as an additional +57% and -7%. Both the 1.08 factor and additional uncertainty have been incorporated into the results presented below.

Results

The results from compiling the inventory data into the three stressor categories are shown below. First, the overall emissions per 1000 liters of ethanol and 3592 kWh of electricity are shown in Figures 7, 8, and 9. Each graph shows the expected value (circle) and the 95% confidence range (vertical bar). Further discussion of the results is provided below.

Table 10 provides a breakdown of the contribution of greenhouse gases for each phase in the six systems producing the same final products (1000 liters ethanol + 3592 kWh).

Figure 7: Comparison of Greenhouse Gases



Figure 8: Comparison of Acid Rain Precursors





Table 10: Fraction of Greenhouse Gases from Each Stage in the Life-Cycle for Each System

	Produce Transport Supply Upstream Ethanol Produce					Produce
System	Feedstock	Feedstock	Water	Natural Gas	Plant	Electricity
	(%)	(%)	(%)	(%)	(%)	(%)
Corn Without	2.09	0.22	0.00	1.83	13.84	82.01
Cogeneration						
Wheat Without	2.10	0.22	0.00	1.13	8.48	88.08
Cogeneration						
Poplar Strong Acid	1.62	0.31	0.04	1.92	14.31	81.79
Without						
Cogeneration						
Poplar Strong Acid	1.82	0.34	0.04	1.67	11.06	85.06
System (I) With						
Cogeneration						
Poplar Strong Acid	4.86	0.92	0.08	12.34	81.80	0.00
System (II) With						
Cogeneration	l					
Poplar Enzymatic	5.81	1.09	0.00	0.00	2.47	90.63
System With						
Cogeneration						

Discussion of Results

Greenhouse Gases

Based on the results presented in Figure 7, the Poplar Strong Acid System (II) with Cogeneration and the Poplar Enzymatic System with Cogeneration both outperform all other four systems from a greenhouse gas emission perspective with approximately one-half the emissions. The primary reason for this is the large electricity-to-ethanol production ratio of these two cogeneration systems which avoids the greenhouse gas emissions associated with electricity production. By comparison, the Poplar Strong Acid System (I) with Cogeneration has a lower electricity-to-ethanol production ratio and results in significantly higher emissions (two times as much). However, large uncertainty exists in the data for the electricity-to-ethanol production ratio of that system, showing that if more electricity could be produced the system's performance could also be significantly better than the three systems without cogeneration. As Table 10 demonstrates, the vast majority of greenhouse gas emissions (over 80%) originates from producing the amount of electricity (3592 kWh) required to match the cogeneration system of the Poplar Strong Acid System (II). It is therefore important to recognize that the assumptions on the source of electricity are very important. Because the Poplar Strong Acid System (II) has the highest electricity-to-ethanol production ratio, it produces the least amount of emissions by off-setting the average electricity grid with relatively clean natural gas powered electricity. Table 10 also demonstrates the low contribution of feedstock production to the total life-cycle (less than 10%) for all systems.

Acid Rain Precursors

Results shown in Figure 8 demonstrate a trend similar to greenhouse gas emissions with respect to systems utilizing cogeneration and systems without cogeneration. The ethanol system providing more electricity to the grid results in lower total emissions of acid rain precursors. However, the difference is even more significant. The system with the highest SO₂ Equivalents emissions (Corn without Cogeneration) produces 400% more acid rain precursor emissions than the lowest emitting system (Poplar Strong Acid System (I) with Cogeneration). Another significant difference is the Poplar Strong Acid System (II) resulting in about half the acid rain precursor emissions of the Poplar Enzymatic System. Again the primary reason for this is the lower use of average-grid electricity which in Alberta operates on 90% coal power resulting in much higher SO₂ emissions than natural gas sources of electricity.

Ground Level Ozone Precursors

Figure 9 shows that the Poplar Strong Acid System (II) with Cogeneration produces about 67-70% less ground-level ozone precursors (NOx + VOCs) than non-cogeneration systems. Again, the difference is largely attributable to the displacement of a significant amount of coal-fired electricity production by the ethanol plant cogeneration. As before, the Poplar Enzymatic System with Cogeneration results in comparatively less advantage due to lower electricity production.

Sensitivity Analysis: Assume All Electricity from Natural Gas Sources

The use of Monte Carlo Analysis allowed for a calculation of uncertainty in the results and also enables one to calculate the contribution of each unit process to the overall uncertainty. The set of assumptions and factors which has the greatest influence on the results of this LCA study relates to producing the electric power which is offset by the ethanol plant cogeneration systems. In the main LCA analysis, this was assumed to be "grid-average" electricity of which a high fraction is produced in coal-fired power plants. Table 10 illustrates the importance of this: for all systems other than the Poplar Strong Acid System (II), over 80% of greenhouse gas emissions result from electricity production. This makes the assumptions around off-setting grid average electricity very significant. One alternative is to assume the excess fraction of the 3592 kWh is produced by natural gas fired turbines in all cases. This would occur by assuming each of the fuel production options installed natural gas-fired generation capable of producing the excess fraction of the 3592 kWh of electricity or by assuming the cogeneration systems off-set marginal grid power provided by natural gas turbines rather than average grid power. The modified results for greenhouse gas emissions are shown in Figure 10. The systems with significant amounts of cogeneration still produce the lowest greenhouse gas emissions due to using significant amounts of biomass (lignin) to reduce fossil fuel combustion. The most significant change when excess electricity is produced with natural gas is the improved performance of the Poplar Enzymatic System with Cogeneration. When natural gas is combusted to produce the electricity for all systems, the Poplar Enzymatic system results in 40% less emissions of greenhouse gases than the Poplar Strong Acid System (II). This is because the Enzymatic System requires no natural gas for the operation of its plant. It operates entirely on the combustion of the lignin co-product from the poplar trees but requires natural gas to produce the extra 1706 kWh of excess electricity to match the total functional unit (1000 liters ethanol + 3592 kWh).



Sensitivity Analysis: Include Fertilizer Production

The analysis completed so far does not include the production of fertilizers required for the growth of the feedstock. The reason for this, is the RMEE system boundary selection method eliminates unit processes considered insignificant to the overall results and instead approximates upstream emissions with an adjustment factor (for this study the adjustment factor was 1.08). To confirm this assumption, the analysis was run with the fertilizer production included. The results are shown in Figure 11 (note these results assume grid-average electricity, not natural gas power). The results show fertilizer production to be insignificant to the results with no change in the conclusions.

Figure 11: Greenhouse Gas Emissions When Including Fertilizer Production with Grid Average Electricity (Uncertainty not available)



Greenhouse Gases

Conclusions

This study has shown that:

- Ethanol production systems utilizing cogeneration to off-set average grid electricity tend to have significantly lower overall emissions than non-cogeneration systems, and the results are very dependent on the systems' ratio of electricity-to-ethanol production. Processes with higher electricity production give lower overall emissions due to the consequent elimination of greenhouse gas emissions from coal-fired grid electricity.
- The results are sensitive to assumptions on the source of electricity, which is off-set by the cogeneration system. A significant fraction of grid average electricity is coal-fired but the off-set savings could be reduced if it was assumed that gas-fired, or hydro was being off-set instead of grid-average power.
- When the electricity off-set by cogeneration is assumed to be produced from natural gas sources, the Poplar Enzymatic System with Cogeneration has the lowest air emissions because it relies the least on fossil-fuels.
- In the life-cycle of producing 1000 liters of ethanol and 3592 kWh of electricity, biomass feedstock production contributes less than 10% of air emissions for all six systems considered.
- Emissions from the production of fertilizers for growing feedstock do not significantly affect the results or conclusions.

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Appendix II Description of the LCA Model

Appendix II provides a brief description of the software model which has been modified and applied throughout this research.

Appendix II – Description of the E3-LCA Model

Introduction

In order to complete this research a model was programmed for simulating life-cycle systems. This model was designed and developed by the author using Visual Basic and Microsoft Access and is called the "E3-LCA Model". The next section provides a brief background of simulation and modeling, followed by a description of how the model for this work was developed.

Simulation and Modeling Background

A computer model is simply an electronic representation of an object, system, or idea [1]. Models can be developed for a number of applications. As identified in *Shannon (1975)* there are at least five common uses of models:

- an aid to thought,
- an aid to communication,
- purposes of training and instruction,
- a tool of prediction, and
- an aid to an experimentation. [1]

For the use in LCA, the first four uses are the most common use of an electronic model. All working towards making better decisions.

Shannon also breaks models into four characteristics for classification:

- 1. static (cross-section) vs. dynamic (time-series),
- 2. deterministic vs. stochastic,
- 3. discrete vs. continuos, and
- 4. iconic vs. analog vs. symbolic. [1]

In LCA, models are typically static that is they take a "snap-shot" in time and make a comparison between options at the same point in time. However, LCA does have the capacity to compare dynamic systems throughout their life-cycle. LCA modeling is also generally deterministic, but as shown in this work stochastic capabilities are emerging. Discrete methods opposed to continuous models are also most common in LCA. Finally, LCA models are symbolic models which utilize mathematical functions to symbolize the real system.

The major advantage of system simulation through modeling before the actual construction of a system is a gain in incite with respect to how the real system may function and compare to alternative systems. Of course caution is required in the use of simulations because they are not the true physical system and by definition can not one-hundred percent accurately reflect the real world [1]. Models can also be very expensive to develop. The research presented here is aimed at reducing these costs by optimizing the use of resources and time on the components of the simulation which have the greatest impact on the decision.

Shannon identifies seven criteria that good simulation models should meet. These are presented in table A.1 along with a description on how the model developed for this research is meeting these criteria.

 Table A.1: Seven Criteria for Good Simulation Models and How This LCA Model

 Meets Them

Criteria [1]	The LCA Model
1. Simple to understand by the user.	The model presents each system symbolically in a flow diagram. This allows visualization of the system opposed to analytical methods which result in often very abstract relationships.
2. Goal or purpose directed.	The process of LCA focuses on defining a clear decision to make. The model is designed to answer this specific question.
3. Robust, in that it does not give absurd answers.	This is a key area of this research. By developing methods for sensitivity analysis, system boundary selection and uncertainty analysis the robustness of LCA modeling increases substantially.
4. Easy for the user to control and manipulate.	The current model is relatively easy to manipulate and control, but will improve as the user interface is further improved upon.
5. Complete on important issues.	The primary objective of the methods of system boundary selection and sensitivity analysis are to help identify the most important issues in the modeling process.
6. Adaptive, with an easy procedure for model modification or updating.	This will advance over time as the user interface is further developed.
7. Evolutionary, in that it should start simply and become more complex, in conjunction with the user.	The LCA model has evolved over five years and will continue to become more powerful in helping environmental and economic decision making.

Description of the E3-LCA Model

Development of the E3-LCA Model began early in 1995 and has evolved over the course of this research to provide an aid in testing the sensitivity analysis, uncertainty analysis, and RMEE system boundary selection methods. The model which has been adapted for this research operates on a Microsoft Access / Visual Basic platform. The system is essentially a referential database with Visual Basic code manipulating tables of data. The final version used in this research had the filename: "E3-LCA Model – July 99.mdb".

Data Storage Structure

The E3-LCA Model is a referential database consisting of 21 tables to store the relevant information for projects, systems, and unit processes. Figure A.1 illustrates the basic structure of the model. A "Project" is defined as a set of systems or options being compared with a specific goal definition and a defined functional unit. As an example, a project comparing automotive fuels would have a collection of systems or options (different fuels) to be compared. Figure A.2 shows the user-interface for projects. Each system in a project consists of a collection of unit processes. These unit processes are connected with flows of inputs and outputs to create a system. Figure A.3 shows the user-interface for systems. Each unit process may have one or more "data sets". A data set defines a given source of data for a unit process. As an example, the refinery unit process may have a number of different data sets defined by location, technology, year, or company. This allows one to run different scenarios by switching data sets. Each data set defines the inputs, outputs and environmental outputs associated with each unit process. Figure A.4 shows the user-interface for individual unit processes. This structure allows the user to clip together unit processes graphically to create systems. These systems can then be modeled to make a comparison.

Calculation of Mean Environmental Outputs

The user selects which system to be modeled and the functional unit to be supplied by the system. The functional unit drives the entire model. As a result, each unit process must be directly or indirectly linked to providing the unit process, otherwise it will not be included in the calculation procedure. The actual procedure for calculating the total environmental outputs is a recursive function which works upstream from the functional unit through the system. This procedure builds tables of input/output flows and environmental outputs. This raw data is then organized into stressor categories for reporting. All of the results are exported to Microsoft Excel files for graphing and further reporting.

Marginal Sensitivity Analysis

Marginal sensitivity analysis is completed by running the model twice for each unit process the user wishes to test sensitivity for. The user selects the unit processes in the system to test and a percentage change to test for. As an example, if the user selects a 1% sensitivity test, then the model will test the sensitivity in results by changing first the inputs by a 1% increase for each unit process being tested independently, and then a 1% increase in environmental outputs. The model then calculates the percent change in total results, resulting from the sensitivity. From this the user can readily identify which unit process data points result in the greatest sensitivity.

Monte Carlo Analysis Routines

To calculate error propagation Monte Carlo Analysis is used. The user defines the standard deviation of each data point and selects the distribution to be applied. Currently two distributions are available: the normal and the beta. The user also selects the number of iterations to make. The model then runs the system, each run selecting a random value for each data point in the system with a defined distribution and standard deviation. The results from each run are stored in a table, which is then exported to Microsoft Excel for statistical analysis.

The algorithms used for selecting random values from the distributions are from Rubinstein (1981) [2]. For the normal distribution, the Box and Muller algorithm has been used. The algorithm is:

"If U₁ and U₂ are independent random variates from (0,1) then the variates $Z_1 = (-2\ln U_1)^{1/2} \cos 2\pi U_2$ $Z_2 = (-2\ln U_1)^{1/2} \sin 2\pi U_2$ are independent standard normal deviates."[2]

Random values from the beta distribution are generated by using an algorithm involving two random variables form the Gamma distribution. The algorithm is as follows:

- "1. Generate Y_1 from G(alpha, 1). (Gamma distribution) 2. Generate Y_2 from G(beta, 1).
- 3. $X = Y_1 / (Y_1 + Y_2)$
- 4. Deliver X."[2]

Uncertainty Reduction Analysis

Uncertainty Reduction Analysis is completed by the user selecting the unit processes to test the effect of eliminating all uncertainty in those unit processes. For each unit process selected, the Monte Carlo Analysis is run for the system. The resulting uncertainty is compared to the baseline uncertainty where no unit process uncertainty has been eliminated. The results of this comparison are exported to Excel.

Relative Mass-Energy-Economic (RMEE) Routines

The RMEE method is built into the model for each run. If the user selects the RMEE cutoff (Z_{RMEE}) to be zero, the entire model is run. If a different cut-off value is selected, then as the model runs through the system, it tests each flow for inclusion in the system based on the mass, energy and economic value defined for the functional unit and each flow in the system. This completely automates the process of applying RMEE to various systems. A table is generated to indicate which flows in the system have been cut by the system boundary and which criteria resulted in the cut (mass, energy or economic).

Random System Generation

For the purpose of testing the RMEE method of system boundary selection and deriving a relationship between system boundary and uncertainty in results, a random system generated was developed. This module would not normally be used in a life-cycle assessment, but is a research tool. The module generates a user-defined number of random systems with a user-specified number of unit processes and type of functional unit. The rules for generating random systems are those defined by Raynolds et al [3].



Figure A.1: Basic Structure of the Life-Cycle Model





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Figure A.4: User Interface for a Unit Process

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Appendix III Data Sources for Fuel Comparison

Appendix III provides a print-out of each data set from the model for the fuel comparison presented in Chapter 6.

Data For: AF - Operate Vehicle

Data Set RFG - Taurus - 1995

Description: NREL's Alternative Fuels Utilization Program - found at Alternative Fuels Data Center - www.afdc.nrel.gov

Emissions are actual measurements.

Ford Taurus is 1995 model year. Data from a federal fleet which is monitored over time.

Desired Products/Services

Output	Amount		Allocation	n Primary Output?	Notes	
AF - Travel km	100	0.0000 km	1	Z		

Material/Service Inputs

Input	Mean	+/-	%	Notes:
AF - Vehicle	0.0005 unit	50	50	100 km / 200,000 km life = 0.0005 of a car's life. Assume 50% uncertainty.
AF - Vehicle Maintance	100.0000 km	50	50	
Reformulated Gasoline	11. 580 0 I	10	10	•

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:	
VOC	Volatile Organic Chem	0.0084 kg	45	45	
NOx	Nitrogen Oxides	0.0084 kg	80	80	
CO2	Carbon Dioxide	26.5377 kg	10	10	
со	Carbon Monoxide	0.0779 kg	45	45	
CH4	Methane	0.0008 kg	25	25	
		_			

Note: +/-% is for the 95% confidence interval of the data.

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Data For: AF - Operate Vehicle

Data Set	E85 -	Taurus -	NREL -	1995
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Description: NREL's Alternative Fuels Utilization Program - found at Alternative Fuels Data Center www.afdc.nrel.gov

Emissions are actual measurements. For ethanol, the ethanol portion is assumed to emit zero CO2.

Ford Taurus is 1994, 95, and 97 model years averaged. Data from a federal fleet which is monitored over time.

Desired Products/Services

Output	Amount	A	llocation	n Primary Output?	Notes	
AF - Travel km	100.	.0000 km	1	¥		

Material/Service Inputs

Input	Mean	+/- %	Notes:
AF - Vehicle	0.0005 unit	50 50	100 km / 200,000 km life = 0.0005 of a car's life. Assume 50% uncertainty.
AF - Vehicle Maintance	100.0000 km	50 50	10 cents per km
Ethanol Blend - E85	15.3200 I	10 10	•

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	6	Notes:	
VOC	Volatile Organic Chem	0.0064 kg	85	85		
NOx	Nitrogen Oxides	0.0081 kg	100	100		
CO2	Carbon Dioxide	5.0884 kg	20	20		
со	Carbon Monoxide	0.0809 kg	50	50		
CH4	Methane	0.0019 kg	70	70		

Note: +/-% is for the 95% confidence interval of the data.

Data For:	AF - Operate	Vehicle
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Data Set Natural Gas - Taurus - Conversion - 1994

Description: NREL's Alternative Fuels Utilization Program - found at Alternative Fuels Data Center www.afdc.nrel.gov

Emissions are actual measurements.

Ford Taurus is 1994 model year with a natural gas conversion kit. Data from a federal fleet which is monitored over time.

Desired Products/Services

Output	Amount	Allocation Primary Output?	Notes
AF - Travel km	100.0000 km	1 🗹	

Material/Service Inputs

Input	Mean	+/- 9	%	Notes:
AF - Vehicle	0.0005 unit	50	50	100 km / 200,000 km life = 0.0005 of a car's life. Assume 50% uncertainty.
AF - Vehicle Maintance	100.0000 km	50	50	
NG	13.5000 m3	15	15	

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- 9	6	Notes:
VOC	Volatile Organic Chem	0.0022 kg	40	40	· · · · · · · · · · · · · · · · · ·
NOx	Nitrogen Oxides	0.0368 kg	115	100	
CO2	Carbon Dioxide	24.2004 kg	15	15	
co	Carbon Monoxide	0.1293 kg	65	65	
CH4	Methane	0.0307 kg	65	65	

Note: +/-% is for the 95% confidence interval of the data.

Data For: AF - Refuel Vehicle

Data Set RFG

Description: California Air Resources Board (CARB) - Ranjit Bhullar 916-323-7370. April, 1999. Number given was 8.4 lbs of VOC per 1000 gallons of fuel dispensed.

Desired Products/Services

Output	Amount	Allocation Pr Ou	Notes	 	
Reformulated Gasoli	1,000.0000 1	1 🗹			
	•				
Material/Service	e inputs Mean	+/- %	1	Notes:	
			<i>I</i> 50	Notes:	

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:
VOC	Volatile Organic Chem	1.0100 kg	50	50

Data For: AF - Refuel Vehicle

Data Set E85

Description: California Air Resources Board (CARB) - Ranjit Bhullar 916-323-7370. April, 1999. Number given was 8.4 lbs of VOC per 1000 gallons of gasoline fuel dispensed.

Desired Products/Services

Output	Amount	Allocation	ry Notes 1?		
Ethanol Blend - E85	1,000.0000 i	1	Ī		
Material/Servic	e Inputs				
Input	Mean	+/- 9	%	Notes:	
AF - Station	0.0000 unit	25	25		
Ethanol Blend - E85	1,000.0000 1	0	0		

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:
voc	Volatile Organic Chem	1.0100 kg	50	50

Data For: AF - Refuel Vehicle

Data Set Natural Gas

Description: Discussions with Dr. Checkel of University of Alberta.

Desired Products/Services

Amount	Allocation Prima Output	-
999.0000 m3	1 🗹	
ice Inputs		
Mean	+/- %	Notes:
1,000.0000 m3	0 0	
	999.0000 m3 ice Inputs Mean	Output 999.0000 m3 1 fice Inputs Mean +/- % +/- %

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:
CH4	Methane	6.5400 kg	50	50 Based on density of natural gas at standard temp and pressure.

Data For:	Refinery
Data Set	Shell Scotford 1993
Description:	Based on Shell's application for approval 1993. This refinery has been designed to produced gasoline, fuel oil, jet fuel, benzene from synthetic crude oil from Alberta oil sands.
	350 permanent employees for plant operation.; 430 according to NPRI
	Assume 20% uncertainty in emissions.

Desired Products/Services

Output	Amount	Allocation	n Prim Outp	•
diesel	1,866,200,000.0000	0.4	E	
Other Refinery Produ	1,120,000,000.0000 (0.2		Includes chemical feedstocks and "other" products
Unleaded Gasoline	1,866,200,000.0000 1	0.4	Z	Varies during year, but on average. Allocation needs to be adjusted.

Material/Service Inputs

Input	Mean	+/-	%	Notes:
Crude Oil	4,528,900,000.0000	50	50	This is entirely synthetic crude oil.
Electricity	401,500,000.0000 kwh	50	50	
NG	302,558.0000 m3	50	50	Based on reported 750 LFE m3/day. Where LFE = liquid fuel equivalent. Converted using 41.8 MJ/LFEm3 and then 37.82 MJ/m3 as has been used with other NG

Air		Mean	+/- %		Notes:
xylene	xylene (m+o+p)	18,537.0000 kg	20	20	
voc	Volatile Organic Chem	3,115,050.0000 kg	20	20	1990 total, reported as "Hydrocarbons"
Toluene	Toluene	22,253.0000 kg	20	20	
SO2	Sulphur Dioxide	462,000.0000 kg	20	20	Reported as SOx for 1990.

PM	Particulate Matter	10,720.0000 kg	20	20	1990
NOx	Nitrogen Oxides	500,100.0000 kg	20	20	1990
Naphthalene	Naphthalene	462.0000 kg	20	20	
Ethylbenzene	Ethylbenzene	5,748.0000 kg	20	20	
Cyclohexane	Cyclohexane	231.0000 kg	20	20	
CO2	Carbon Dioxide	0,000,000.0000 kg	20	20	
Biphenyl	Biphenyl	409.0000 kg	20	20	
Benzene	Benzene	13,975.0000 kg	20	20	
124-Trimethylben	1,2,4-Trimethylbenzen	1,824.0000 kg	20	20	

Data For: Transport Crude Oil

Data Set Monenco 1992

Description: Based on Monenco full fuel cycle study, Appendix G. NOTE: This data set is an exact copy of "Crude Oil Transport - Pipeline".

Desired Products/Services

Output	Amount	Allocation Primar y Output?	Notes
Crude Oil	1,000.0000 i	1 🗹	

Material/Service Inputs

Input	Mean		+/-	%	Notes:	t
Crude Oil	1,000.0000	1	0	0		
Electricity	11.3500	kWh	50	50		
Pipeline	0.0001	unit	-1	-1		

Environmental Outputs (Releases per amount of primary output)

Data For: AF - Produce Crude Oil

Data Set Aggregated - Syncrude Suncor Monenco

Description: Data set generated by combination of Syncrude, Suncor, and Monenco data sets.

Desired Products/Services

Output	Amount		Allocation P C	rimary Dutput?	Notes	
Crude Oil		1.0000 i	1 5	Z		

Material/Service Inputs

Input	Mean	+/-	%	Notes:	
Electricity	0.0971 kWh	-1	-1		· · · · · · · · · · · · · · · · · · ·
NG	0.0884 m3	-1	-1		

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:	
VOC	Volatile Organic Chem	0.0011 kg	-1	-1	
SO2	Sulphur Dioxide	0.0122 kg	-1	-1	
РМ	Particulate Matter	0.0004 kg	-1	-1	
NOx	Nitrogen Oxides	0.0014 kg	-1	-1	
CO2	Carbon Dioxide	0.6832 kg	-1	-1	
со	Carbon Monoxide	0.0015 kg	-1	-1	
CH4	Methane	0.0159 kg	50	50	

Note: +/-% is for the 95% confidence interval of the data.

Data For: AF - Transport MTBE

Data Set 1000 km

Description: Deluchi / AP-42 / Mobile 5a

Desired Products/Services

Output	Amount	Allocation Primary Output?	Notes
MTBE	1,000.0000 (1 🗹	

Material/Service Inputs

Input	Mean	+/-	%	Notes:	
diesel	30.6000 1	50	50		
MTBE	1,000.0000 1	0	0		

Air		Mean	+/- %	Notes:	
VOC	Volatile Organic Chem	0.1010 kg	50	50	<u> </u>
SO2	Sulphur Dioxide	0.0250 kg	50	50	
PM10	10u Particulate Matter	0.0490 kg	50	50	
NOx	Nitrogen Oxides	0.3370 kg	50	50	
N2O	Nitrous Oxide	0.0022 kg	50	50	
CO2	Carbon Dioxide	89.0600 kg	50	50	
со	Carbon Monoxide	0.5600 kg	50	50	;
CH4	Methane	0.0049 kg	50	50	

Data For:	Produce	MTBE
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Data Set Aggregated - EnviroFuels, ABC

Description: Aggregated set of AB EnviroFuels 1 and 2, and Alberta BioClean Project data.

See individual data sets for more detail. Data sets combined using a t-distribution.

Assume 25% uncertainty where not calculated by t-distribution.

Desired Products/Services

Output	Amount		Allocation	Primary Output?	Notes	
Isobutane		0.0311 1	1			
MTBE		1.0000 1	1	₹.		

Material/Service Inputs

Input	Mean	+/-	%	Notes:
Butane	0.0013 m3	0	0	
Chlorine	0.0000 kg	25	25	
Dimethyldisulphide	0.0001 kg	25	25	
Electricity	0.0603 kwh	0	0	
Methanol	0.3474 1	0	0	
NG	0.0403 m3	0	0	
Potassium hydroxi de (0.0003 kg	25	25	
Sodium hydroxid e (50	0.0004 kg	25	25	
Sulphuric Acid (98%)	0.0001 kg	25	25	
Tetrachloroethylene	0.0001 kg	25	25	

Air		Mean	+/- %	5	Notes:
sylene	xylene (m+o+p)	0.0000 kg	25	25	1
/0C	Volatile Organic Chem	0.0000 kg	0	0	2
etrachloroethyle	Tetrachloroethylene	0.0000 kg	25	25	1
602	Sulphur Dioxide	0.0000 kg	0	0	2
lOx	Nitrogen Oxides	0.0004 kg	0	0	2
ITBE	Methyl tert-butyl ether	0.0000 kg	25	25	1
lethanol	Methanol	0.0000 kg	25	25	1
:02	Carbon Dioxide	0.3110 kg	0	0	2
Ö	Carbon Monoxide	0.0001 kg	25	25	1
1	Chlorine	0.0000 kg	25	25	1
H4	Methane	0.0002 kg	25	25	1

Note: +/-% is for the 95% confidence interval of the data.

Data For: AF - Transport Fuel

Data Set RFG

Description: Deluchi for fuel consumption factor, Mobile 5a for emission factors. See "Data Set Calcs - Diesel System.xls - Transport Fuel" for calculation details.

Desired Products/Services

Output	Amount	Allocation Primary Output?	Notes
Reformulated Gasoli	1,000.0000 i	1 🗹	

Material/Service Inputs

Input	Mean	+/-	%	Notes:
diesel	1.5300	25	25	
Reformulated Gasoline	1,000.0000 i	0	0	
Truck - Diesel - Semi T	0.0000 unit	50	50	

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:
VOC	Volatile Organic Chem	0.0050 kg	25	25
SO2	Sulphur Dioxide	0.0013 kg	25	25
PM	Particulate Matter	0.0024 kg	25	25
٩Ox	Nitrogen Oxides	0.0170 kg	25	25
02	Carbon Dioxide	4.4530 kg	25	25
0	Carbon Monoxide	0.0280 kg	25	25
CH4	Methane	0.0003 kg	25	25

Data For: Natural Gas - Transport Service - Pipeline

Data Set Nova Gas 1996

Description: Nova Gas Transmission of Nova Chemicals Inc. Voluntary Climate Change Challenge and Registry (VCR) report for 1996.

Desired Products/Services

Output	Amount	Allocation Primary Output?	Notes
NG Transport	1,000,000.0000 m3i	k 1 ∑	

Material/Service Inputs

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:
NOx	Nitrogen Oxides	3.2200 kg	25	25
CO2	Carbon Dioxide	44.9000 kg	25	25
CH4	Methane	19.4000 kg	25	25

Data For: Upstream Natural Gas

Data Set Monenco 1992 Aggregated

Description: Extracted from Monenco 1994 Full Fuel Cycle Emissions report, appendix G, 1992 data. From table G-1: assumes allocation by volume between propane and natural gas for the gas industry. Reports natural gas to be an input to the gas industry (6,195e6 std. m3), this has been subtracted from the production amount reported, to avoid loop.

System Boundaries Include: exploratory drilling, development drilling, processing, pipeline transport, flaring.

Desired Products/Services

Output	Amount	Allocation P O	rimary utput?	Notes
NG	88,387.5000 m3	1 5	Proc 9456 6195 subt	orted "Marketable Gas ducts - Natural Gas Deliveries" is 82.5e6 std. m3 and an input of 5e6 m3 to produce it. Have tracted these two values to get output.

Material/Service Inputs

Input	Mean	+/- %	6	Notes:
diesel	20.0000 1	50	50	
Electricity	3,847.0000 kWh	50	50	Assume Alberta grid.

Environmental Outputs (Releases per amount of primary output)

	Mean	+/- %	Notes:
Volatile Organic Chem	69.0000 kg	50	50
Sulphur Dioxide	183.0000 kg	50	50
Nitrogen Oxides	137.0000 kg	50	50 Reported as NO2.
Carbon Dioxide	19,153.0000 kg	50	50
Methane	323.0000 kg	50	50
	Sulphur Dioxide Nitrogen Oxides Carbon Dioxide	Volatile Organic Chem69.0000 kgSulphur Dioxide183.0000 kgNitrogen Oxides137.0000 kgCarbon Dioxide19,153.0000 kg	Volatile Organic Chem 69.0000 kg 50 Sulphur Dioxide 183.0000 kg 50 Nitrogen Oxides 137.0000 kg 50 Carbon Dioxide 19,153.0000 kg 50

Note: +/-% is for the 95% confidence interval of the data.

Data For: AF - Transport Fuel

Data Set E85

Description: Deluchi for fuel consumption factor, Mobile 5a for emission factors. See "Data Set Calcs - Diesel System.xls - Transport Fuel" for calculation details.

Desired Products/Services

Output	Amount	Allocation Primary Output?	Notes
Ethanol Blend - E85	1,000.0000 1	1 🗹	

Material/Service Inputs

Input	Mean	+/-	%	Notes:
diesel	1.4400 1	25	25	
Ethanol Blend - E85	1,000.0000 1	0	0	
Truck - Diesel - Semi T	0.0000 unit	50	50	

Air		Mean	+/- %	Notes:
VOC	Volatile Organic Chem	0.0048 kg	25	25
SO2	Sulphur Dioxide	0.0012 kg	25	25
РМ	Particulate Matter	0.0023 kg	25	25
NOx	Nitrogen Oxides	0.0158 kg	25	25
N2O	Nitrous Oxide	0.0001 kg	25	25
CO2	Carbon Dioxide	4.1900 kg	25	25
со	Carbon Monoxide	0.0264 kg	25	25

Data For:	Transport Ethanol
Data Set	Ontario - 3000 km - Rail
Description:	Deluchi - PIAD LCVA Database

Desired Products/Services

Output	Amount	Allocation Prime Outp	•
Ethanol	1,000.0000 1	1 🗹	
Material/Ser	vice Inputs		
Material/Ser Input	vice Inputs Mean	+/- %	Notes:
		+/- % 25 25	Notes:

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:
VOC	Volatile Organic Chem	0.1140 kg	25	25
NOx	Nitrogen Oxides	0.4670 kg	25	25
N2O	Nitrous Oxide	0.0015 kg	25 2	25
CO2	Carbon Dioxide	55.0000 kg	25 2	25
со	Carbon Monoxide	0.1640 kg	25 2	25
CH4	Methane	0.0119 kg	25 2	25

Data For: Transport Natural Gas to Ontario

Data Set Default

Description:

Desired Products/Services

Output	Amount	Allocation	n Prima Outpu	•	
NG	1.0000 m3	1			
Material/Serv					
Input	Mean	+/-	%	Notes:	
NG	1.0000 m3	0	0		-
NG Transport	3,000.0000 m3km	10	10		

Environmental Outputs (Releases per amount of primary output)

Data For: Transport Ethanol Data Set Alberta - 300 km - Truck Description:

Desired Products/Services

Output	Amount	Allocation Primary Output?	Notes	
Ethanol	1,000.0000 1	1 🗹		

Material/Service Inputs

Input	Mean	+/-	%	Notes:
diesel	8.5320 1	25	25	· · · · · · · · · · · · · · · · · · ·
Ethanol	1,000.0000 1	o	o	

Air		Mean	+/- %	Notes:
VOC	Volatile Organic Chem	0.0280 kg	25	25
SO2	Sulphur Dioxide	0.0071 kg	25	25
РМ	Particulate Matter	0.01 4 0 kg	25	25
NOx	Nitrogen Oxides	0.0940 kg	25	25
N2O	Nitrous Oxide	0.0006 kg	25	25
CO2	Carbon Dioxide	24.8300 kg	25	25
со	Carbon Monoxide	0.1560 kg	25	25
CH4	Methane	0.0014 kg	25	25

Data For: Corn Ethanol Conversion

Data Set Commercial Alcohols - Chattam

Description: Inputs and outputs supplied by Matt Janes of Commercial Alcohols in 1995, prior to actual operation of Chattam plant. Emissions have been calculated based only on the combustion of natural gas in an industrial size

boiler. Emissions here do not include other process emissions which may occur, nor fugitive emissions.

Allocation completed by market value, see SBS spreadsheet.

Desired Products/Services

Output	Amount	Allocation Prim Outp	-
CO2	97,000,000.0000 kg	0.117	Carbon dioxide is sold to bottling industry.
DDGS	127,000,000.0000 kg	0.338 🗔	
Ethanol	150,000,000.0000 (0.545 👻	Is the annual production of ethanol, includes 120 M liters of fuel grade and 30 M liters of industrial grade ethanol.

Material/Service Inputs

Input	Mean		+/-	%	Notes:
Ammonia	840,000.0000	kg	50	50	
Com	380,000,000.0000	kg	50	50	
Electricity	2,000,000.0000	kwh	50	50	
Enzyme - alpha-amyla	130,000.0000	kg	50	50	
Enzyme - gluso-amyla	500,000.0000	kg	50	50	
NG	69,700,000.0000	m3	50	50	
Sodium hydroxid e (50	840,000.0000	kg	50	50	not sure if 50% concentration has been specified.
Sulphuric Acid (70%)	400,000.0000	kg	50	50	not sure if 70% concentration has been specified
Water	2,200,000,000.0000	1	50	50	

Environmental Outputs (Releases per amount of primary output)

VOC Volatile Organic Chem 3,400.0000 kg 50 50 SO2 Sulphur Dioxide 773.0000 kg 50 50 PM10 10u Particulate Matter 16,800.0000 kg 50 50 NOx Nitrogen Oxides 114,000.0000 kg 50 50 N2O Nitrous Oxide 525.0000 kg 50 50 CO2 Carbon Dioxide 9,000,000.0000 kg 15 15 CO Carbon Monoxide 42,800.0000 kg 50 50 CH4 Methane 3,690.0000 kg 50 50	Air	Mean	+/- %	Notes:
PM10 10u Particulate Matter 16,800.0000 kg 50 50 NOx Nitrogen Oxides 114,000.0000 kg 50 50 N2O Nitrous Oxide 525.0000 kg 50 50 CO2 Carbon Dioxide 9,000,000.0000 kg 15 15 CO Carbon Monoxide 42,800.0000 kg 50 50	/OC Volatile Organic Cherr	n 3,400.0000 kg	50	50
NOx Nitrogen Oxides 114,000.0000 kg 50 50 N2O Nitrous Oxide 525.0000 kg 50 50 CO2 Carbon Dioxide 9,000,000.0000 kg 15 15 CO Carbon Monoxide 42,800.0000 kg 50 50	SO2 Sulphur Dioxide	773.0000 kg	50	50
N2O Nitrous Oxide 525.0000 kg 50 50 CO2 Carbon Dioxide 9,000,000.0000 kg 15 15 CO Carbon Monoxide 42,800.0000 kg 50 50	PM10 10u Particulate Matter	16,800.0000 kg	50	50
CO2 Carbon Dioxide 9,000,0000 kg 15 15 CO Carbon Monoxide 42,800.0000 kg 50 50	NOx Nitrogen Oxides	114,000.0000 kg	50	50
CO Carbon Monoxide 42,800.0000 kg 50 50	N2O Nitrous Oxide	525.0000 kg	50	50
	CO2 Carbon Dioxide	9,000,000.0000 kg	15	15
CH4 Methane 3.690.0000 kg 50 50	CO Carbon Monoxide	42,800.0000 kg	50	50
	CH4 Methane	3,690.0000 kg	50	50

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Note: +/-% is for the 95% confidence interval of the data.

Data For: Corn Transport

Data Set Mixed - 60km

Description: Uses Deluchi for fuel consumption and Mobile 5a for emissions. Assumes distance of 60km.

Desired Products/Services

Output	Amount	Allocation Primary Output?	Notes
Corn	1,000.0000 kg	1 🗹	
Material/Ser	vice Inputs		
Input	Mean	+/- % 1	Notes:

Corn 1,000.0000 kg 0 0 diesel 2.1600 i 50 50			±7,€	/0	
diesel 2.1600 i 50 50	Corn	1,000.0000 kg	0	0	
	diesel	2.1600 /	50	50	

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:
VOC	Volatile Organic Chem	0.0071 kg	50	50
SO2	Sulphur Dioxide	0.0018 kg	50	50
PM10	10u Particulate Matter	0.0034 kg	50	50
NOx	Nitrogen Oxides	0.0238 kg	50	50
N2O	Nitrous Oxide	0.0002 kg	50	50
CO2	Carbon Dioxide	6.2843 kg	50	50
со	Carbon Monoxide	0.0396 kg	50	50
CH4	Methane	0.0003 kg	50	50

Data For: Corn Storage and Handling

Data Set Ontario

Description: [602] - Ontario report.

This unit process also includes drying of grain. Assumes all drying is down using propane as the fuel.

Desired Products/Services

Output	Amount	Allocation Primary Notes Output?			
Corn	1,000.0000 kg	1	¥		
Material/Ser	vice Inputs Mean	+/- 9	%	Notes:	
Corn	1,000.0000 kg	0	0		
LPG	32.9500 1	50	50	Used in drying the grain.	

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:
VOC	Volatile Organic Chem	0.0017 kg	50 9	50
PM10	10u Particulate Matter	0.0016 kg	50 9	50
NOx	Nitrogen Oxides	0.0223 kg	50 9	50
N2O	Nitrous Oxide	0.0015 kg	50 9	50
CO2	Carbon Dioxide	52.6432 kg	50 9	50
со	Carbon Monoxide	0.0076 kg	50 8	50
CH4	Methane	0.0003 kg	50 5	50

Note: +/-% is for the 95% confidence interval of the data.

Data For: Ontario Corn Harvest

Data Set Mixed Sources

Description: [602] - Corn Production, Utilization and Env. Assessment - Ontario data

Desired Products/Services

Output	Amount	Allocation Primary Notes Output?
Com	6,660.0000 kg	1 🗹
Material/Ser	vice Inputs	
Input	Mean	+/- % Notes:
Corn - Grown	1.0000 ha	50 50

Environmental Outputs (Releases per amount of primary output)

Data For:	Ontario	Corn Farm
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Data Set Mixed Sources

Description: Uses a collection of data sources from various studies on corn ethanol.

One key source is:

'Corn Production, Utilization and Environmental Assessment - A Review' Agriculture and Agri-Food Canada, Ottawa, 1996

Desired Products/Services

Output	Amount		Allocation	Primary Output?	Notes	
Corn - Grown		1.0000 ha	1	Z		

Material/Service Inputs

Input	Mean		+/- %		Notes:
Corn - Maintain Farm	1.0000	ha	50	50	
Com - Plant Farm	1.0000	ha	0	0	
Electricity	160.0000	kWh	50	50	Based on average use of elec. for agriculture in Canada and total hectares farmed. See excel spreadsheet.
Water	4,662,000.0000	i	15	15	

Environmental Outputs (Releases per amount of primary output)

Data For: Ontario Corn Maintenance

Data Set Ontario

Description: [602] - Ontario data. Assumes Moldboard plow for tillage.

Desired Products/Services

Output	Amount	nt Allocation Primary Notes Output?					
Corn - Maintain Farm		1.0000 ha	1	Z	Farm maintenance operations.		

Material/Service Inputs

Input	Mean	+/- 9	%	Notes:
diesel	14.4030	50	50	Diesel fuel for tillage only, combusted in a tractor. This value does NOT include application of fertilizer or planting.
Fertilizer - K20	47.0000 kg	50	50	Ontario data - 1991
Fertilizer - N	115.0000 kg	50	50	Ontario data - 1991: Made up of three sources: Urea, U.A.N., Anhydrous
Fertilizer - P2O5	77.0000 kg	50	50	Ontario data - 1991

Air		Mean	+/- %	Notes:
/0C	Volatile Organic Chem	0.0475 kg	50	50
02	Sulphur Dioxide	0.0120 kg	50	50
M10	10u Particulate Matter	0.0230 kg	50	50
Ox	Nitrogen Oxides	0.4960 kg	50	50
20	Nitrous Oxide	0.0011 kg	50	50

CO2	Carbon Dioxide	42.0572 kg	50	50
со	Carbon Monoxide	0.1764 kg	50	50
CH4	Methane	0.0023 kg	50	50

Note: +/-% is for the 95% confidence interval of the data.

Data For: Ethanol Production - Lignocellulose

Data Set Enzymatic - NREL 1998 - AB Elec Credit

NREL study: "Environmental Life Cycle Implications of the Use of California Biomass in the Production of Fuel Oxygenates" Vol. I, Sept. 1998 (Draft Final Report) Emission factors from AP-42. Process from NREL modeling and experience.

Desired Products/Services

Output	Amount		Al	location	n Primary Output?	Notes	
CO2		0.6900	kg	0.2			
Electricity		1.8861	kWh	0			
Ethanol		1.0000	1	0.8	$\mathbf{\overline{Z}}$		
Gypsum		0.0070	kg	0			
Lignin		2.4330	kg	0			

Material/Service Inputs

Mean	+/- %		Notes:
0.0060 kg	50	50	
4.2690 kg	50	50	
0.1470 kg	50	50	economic value is a guess only
0.0107 1	50	50	
0.0030 kg	50	50	
0.0260 kg	50	50	
0.2900 kg	50	50	
	0.0060 kg 4.2690 kg 0.1470 kg 0.0107 i 0.0030 kg 0.0260 kg	0.0060 kg 50 4.2690 kg 50 0.1470 kg 50 0.0107 i 50 0.0030 kg 50 0.0260 kg 50	0.0060 kg 50 50 4.2690 kg 50 50 0.1470 kg 50 50 0.0107 i 50 50 0.0030 kg 50 50 0.0260 kg 50 50

Air		Mean	+/- %	Notes:	
VOC	Volatile Organic Chem	0.0002 kg	50	50	
8/2/00		<u></u>	<u> </u>	· · · · · · · · · · · · · · · · · · ·	

Description: This data has been adjusted to give an emission credit for the electricity produced. It is assumed the electricity off-sets AB grid average.

Sulphur Dioxide	-0.0057 kg	50	50	
10u Particulate Matter	0.0031 kg	50	50	
Nitrogen Oxides	-0.0015 kg	50	50	
Nitrous Oxide	0.0001 kg	50	50	
Carbon Dioxide	-2.0007 kg	15	15	
Carbon Monoxide	0.0008 kg	50	50	
Methane	-0.0006 kg	50	50	
	10u Particulate Matter Nitrogen Oxides Nitrous Oxide Carbon Dioxide Carbon Monoxide	10u Particulate Matter0.0031 kgNitrogen Oxides-0.0015 kgNitrous Oxide0.0001 kgCarbon Dioxide-2.0007 kgCarbon Monoxide0.0008 kg	OutputStoredStored10u Particulate Matter0.0031 kg50Nitrogen Oxides-0.0015 kg50Nitrous Oxide0.0001 kg50Carbon Dioxide-2.0007 kg15Carbon Monoxide0.0008 kg50	10u Particulate Matter0.0031 kg5050Nitrogen Oxides-0.0015 kg5050Nitrous Oxide0.0001 kg5050Carbon Dioxide-2.0007 kg1515Carbon Monoxide0.0008 kg5050

Data For:	Transport	Biomass
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Data Set Diesel Truck - 60km

Description: Uses Deluchi for fuel consumption and Mobile 5a for emissions. Assumes transport distance of 60km.

Desired Products/Services

Output	nt Amount Allocation Primary Note Output?		•	
Biomass (75% cellul	1,000.0000 kg	1	Z	
Material/Service	e Inputs			
Input	Mean	+/- 9	6	Notes:
Biomass (75% cellulos	1,046.0000 kg	10	10	Takes into account a 4.6% hauling loss. The uncertainty is a guess.
tiesel	2.1600 !	50	50	

Air		Mean	+/- %	Notes:	
VOC	Volatile Organic Chem	0.0071 kg	50	50	
SO2	Sulphur Dioxide	0.0018 kg	50	50	
PM10	10u Particulate Matter	0.0034 kg	50	50	
NOx	Nitrogen Oxides	0.0238 kg	50	50	
N2O	Nitrous Oxide	0.0020 kg	50	50	
CO2	Carbon Dioxide	6.2843 kg	50	50	
со	Carbon Monoxide	0.0396 kg	50	50	
CH4	Methane	0.0003 kg	50	50	

Data For:	Harvest	Poplar	Plantation
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Data Set Drayton Valley Region

Description: Data completed by K. Finigan of Pembina Institute by interviewing potential farmers/foresters in Drayton Valley region.

Data is on a dry basis for all aboveground biomass. Collected May 1998.

Desired Products/Services

Output	Amount	Allocation Prime Outpe	•
Biomass (75% cellul	6,854.0000 kg	1 🗹	Dry - above ground biomass
Material/Service	e Inputs		
Input	Mean	+/- %	Notes:
Poplar Plantation Land	1.0000 ha	50 50	

Environmental Outputs (Releases per amount of primary output)

Data For: Maintain Poplar Plantation

Data Set NREL 1997

Description: Plantation assumed to be located in North-Central Iowa/South-Central Minnesota region of U.S. Data obtained from researchers at Oak Ridge National Laboratory (ORNL).

Based on annual production. Plantation operates on a 7 year rotation, meaning a field of poplars is harvested once every 7 years.

This unit process also includes the diesel consumption in harvesting the crop.

Desired Products/Services

Output	Amount		Allocation	Primary Output?	Notes
Poplar Plantation La		1.0000 ha	1	2	

Material/Service Inputs

Input	Mean		+/-	%	Notes:
diesel	82.7400	I	50	50	Based on considering all the operations and machinery used in the 7 year rotation, averaged over 30 years of operation.
Electricity	160.0000	kWh	50	50	Based on average use of elec. for agriculture in Canada and total hectares farmed. See excel spreadsheet.
Fertilizer - K2O	5.6000	kg	50	50	Based reported 39.2 kg/ha for 7 year rotation. Occurs in year one.
Fertilizer - N	14.2900	kg	50	50	Based on reported 100 kg/ha once in 7 year rotation, in year four.
Fertilizer - P2O5	7.3329	kg	50	50	Based on reported 22.4 kg/ha as P. This has been converted to P2O5 using the molecular weight of P2O5. Occurs in year one.

Air		Mean	+/- %		Notes:
VOC	Volatile Organic Chem	0.2731 kg	50	50	Based on emissions from *dies tractor*.

Sulphur Dioxide	0.0689 kg	50	50	
10u Particulate Matter	0.1321 kg	50	50	
Nitrogen Oxides	2.8496 kg	50	50	
Nitrous Oxide	0.0061 kg	50	50	
Carbon Dioxide	241.6068 kg	50	50	
Carbon Monoxide	1.0136 kg	50	50	
Methane	0.0134 kg	50	50	
	10u Particulate Matter Nitrogen Oxides Nitrous Oxide Carbon Dioxide Carbon Monoxide	10u Particulate Matter0.1321 kgNitrogen Oxides2.8496 kgNitrous Oxide0.0061 kgCarbon Dioxide241.6068 kgCarbon Monoxide1.0136 kg	10u Particulate Matter0.1321 kg50Nitrogen Oxides2.8496 kg50Nitrous Oxide0.0061 kg50Carbon Dioxide241.6068 kg50Carbon Monoxide1.0136 kg50	10u Particulate Matter0.1321 kg5050Nitrogen Oxides2.8496 kg5050Nitrous Oxide0.0061 kg5050Carbon Dioxide241.6068 kg5050Carbon Monoxide1.0136 kg5050

Note: +/-% is for the 95% confidence interval of the data.

Data For: Alberta Electricity

Data Set AIS 1995

Description: Alberta average grid. Includes coal, natural gas and hydro sources. Supplied by TransAlta Utilities, 1995 data.

Assume +/- 10% uncertainty.

Desired Products/Services

Output	Amount	Allocation Primary Output?	Notes
Electricity	1,000.0000 kW	h 1 🗹	

Material/Service Inputs

Environmental Outputs (Releases per amount of primary output)

Air		Mean	+/- %	Notes:	
VOC	Volatile Organic Chem	0.0250 kg	10	10	
S02	Sulphur Dioxide	3.0980 kg	10	10	
РМ	Particulate Matter	0.2340 kg	10	10	
NOx	Nitrogen Oxides	1.8880 kg	10	10	
N2O	Nitrous Oxide	0.0260 kg	10	10	
CO2	Carbon Dioxide	1,076.3270 kg	10	10	
со	Carbon Monoxide	0.1430 kg	10	10	
CH4	Methane	0.3550 kg	10	10	

Note: +/-% is for the 95% confidence interval of the data.