ENGINEERING FOR SUSTAINABLE DEVELOPMENT FOR BIO-DIESEL PRODUCTION

A Thesis

by

DIVYA NARAYANAN

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

May 2007

Major Subject: Chemical Engineering

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Approved by:

Chair of Committee,	M Sam Mannan
Committee Members,	Ramesh Talreja
	Mahmoud El-Halwagi
Head of Department,	N.K.Anand

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ABSTRACT

Engineering for Sustainable Development for Bio-Diesel Production. (May 2007)

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Chair of Advisory Committee: Dr. M. Sam Mannan

Engineering for Sustainable Development (ESD) is an integrated systems approach, which aims at developing a balance between the requirements of the current stakeholders without compromising the ability of the future generations to meet their needs. This is a multi-criteria decision-making process that involves the identification of the most optimal sustainable process, which satisfies economic, ecological and social criteria as well as safety and health requirements. Certain difficulties are encountered when ESD is applied, such as ill-defined criteria, scarcity of information, lack of process-specific data, metrics, and the need to satisfy multiple decision makers. To overcome these difficulties, ESD can be broken down into three major steps, starting with the Life Cycle Assessment (LCA) of the process, followed by generation of non-dominating alternatives, and finally selecting the most sustainable process by employing an analytic hierarchical selection process. This methodology starts with the prioritization of the sustainability metrics (health and safety, economic, ecological and social components). The alternatives are then subjected to a pair-wise comparison with respect to each Sustainable Development (SD) indicator and prioritized depending on their performance. The SD indicator priority score and each individual alternative's performance score together are used to determine the most sustainable alternative.

The proposed methodology for ESD is applied for bio-diesel production in this thesis. The results obtained for bio-diesel production using the proposed methodology are similar to the alternatives that are considered to be economically and environmentally favorable by both researchers and commercial manufacturers; hence the proposed methodology can be considered to be accurate. The proposed methodology will also find wide range of application as it is flexible and can be used for the sustainable development of a number of systems similar to the bio-diesel production system; it is also user friendly and can be customized with ease. Due to these benefits, the proposed methodology can be considered to be a useful tool for decision making for sustainable development of chemical processes.

DEDICATION

To Swami Ayappan for his endless blessing.

To Amma and Appa for their endless love, support and encouragement.

To Suraj, Bell Thatha and JP for their unconditional love.

To Sharan for his constant love, patience and motivation.

To Dr. Mannan and the members of the Mary K O'Connor Process Safety Center for the inspiration.

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1 INTRODUCTION

1.1 Overview

The advances in the chemical industry have intensified its impact on not only the environment but also on the economy and the society. Though some of these impacts are immediately recognized and some have a cumulative and global effect. Thus it becomes important to ensure a Sustainable Development (SD) of these processes not with respect to just environmental impact, resource consumption but also with respect to societal and economic impacts. Hence chemical companies have begun to assign strategic importance to SD by incorporating them into their decision making. In order to ensure a complete SD appropriate tools and techniques are required for evaluating available choices and identifying the most sustainable alternative.

Engineering for Sustainable Development (ESD) is an integrated systems approach, which aims at developing a balance between the requirements of the current stake-holders without compromising the ability of the future generations to meet their needs. This is a Multi Criteria Decision-Making (MCDM) problem that involves the identification of the most optimal sustainable process, which satisfies certain economical, ecological and social criteria as well as safety and health requirements. Certain difficulties are encountered when ESD is applied such as ill-defined criteria,

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This thesis follows the style of Journal of Bioresource Technology.

scarcity of information, lack of process-specific data and the need to satisfy the requirements of multiple decision makers. In order to overcome these difficulties, a decision making technique has been developed to quantify the sustainability of process alternatives in order to identify the most suitable one. This method is a combination of a number of decision making techniques and process quantifying methodologies. It incorporates Life Cycle Assessment (LCA) for studying the process as a whole, SD metrics and Risk Assessment Matrix (RAM) for quantifying the process impacts, MCDM techniques for the comparison and identification of the most sustainable alternative. The feasibility and effectiveness of the proposed method is shown by applying it to the selection of the most sustainable process for biodiesel production.

1.2 Sustainable Development (SD)

The original concept of SD, defined over 15 years ago by a U.N Commission, suggested pursuing development in a way that respects both human needs and global ecosystems, assuring a quality of life for future generations (WCED, 1987). The chemical industry has made significant technological progress over the last decade in terms of improvement in environmental performance and production efficiency and the industry has started realizing the strategic importance of improving the sustainability of its activities due to its contribution to improving both tangible and intangible assets. In order to remain competitive, most existing processes require constant improvement through retrofitting while new processes need to satisfy strict regulations with respect to environmental impact and process safety. Thus in order to increase productivity, optimize resource and energy consumption, minimize waste generation and meet the requirements of process safety and process controllability and meet societal requirements and constraints, SD must be made an integral part of the process design and development stage of chemical processes. In this research the topic of SD is addressed with respect to the development of a process to manufacture bio-diesel.

Since SD includes the analysis of various contradictory implications of a process as well as the requirements of multiple decision makers, it can be classified as a MCDM problem. In order to solve this MCDM problem, certain analytical tools, adapted from the field of operations research and management science, are modified and used in this research work. The tools used are the Life Cycle Assessment (LCA) tool and the Analytical Hierarchical Process (AHP) tool. LCA is used to define the system boundaries and to identify the SD indicators within the defined sub-systems while AHP is used to compare the alternatives for identifying the most sustainable option. The combination of these two analytical methods has been employed in developing a decision making tool for the SD of bio-diesel production process.

1.3 Bio-diesel

High energy costs, increasing demands, concerns about petroleum reserves and greater realization of the environmental impacts of fossil fuels have increased the interest in bio-fuels. For bio-diesel to be a suitable substitute for fossil fuels, its sustainability as a fuel has to be established. This translates to establishing that bio-fuels have superior environmental benefits while being economically competitive with fossil fuel, and that they can be produced in sufficient quantities to satisfy the existing energy demand while providing a net energy gain over the energy sources used in producing them. This analysis is analogous to performing a SD on the life cycle of a bio-fuel system. The bio-fuel considered here for the SD is bio-diesel. LCA methodology is used for defining the system boundaries for the bio-diesel system which includes a complete cradle to grave analysis of bio-diesel inclusive of the raw materials, the chemical reactants, the process conditions, the by-products, the waste treatment options as well as the disposal of the wastes, excess reactants and the used end product. Then SD indicators are used to quantify the impact bio-diesel has on the environment, economy, society and safety of the surroundings over its lifetime. The analytical comparison tool, AHP is used to prioritize the available alternatives depending on their degree of sustainability. Finally the end result of the analysis is a complete bio-diesel system that is sustainable from its cradle to its grave.

2 SUSTAINABLE DEVELOPMENT (SD)

The large impact of the modern chemical and energy industry on the environment, society and economy is evident and has given rise to scope for extensive research and discussion on quantifying and balancing these impacts. In general, the present interaction of the modern society with the ecological system is unsustainable, that is, if the current rate of depletion of natural resources, growth of economic imbalance and environmental pollution continues it will result in serious irreparable consequences and imbalances in the future. To emphasize on this further, it is required to define SD. There are a number of definitions, the most widely used one is the one described by the Brundtland Commission of 1987, which defines SD as the "*Development that meets the needs of the present generation without compromising the ability of the future generations to meet their own needs*". This quote makes clear that the development of new technologies has to take into account economical and social issues (present generations) and long term and large scale environmental issues (future generations).

Another popular definition is " A *sustainable product or process is one that constrains resource consumption and waste generation to an acceptable level, makes a positive contribution to the satisfaction of human needs, and provides enduring economic value to the business enterprise*" (Robert, 1997). The determination of an "acceptable level" represents a technical challenge, but is common to assert that resource utilization should not deplete existing capital, that is, resources should not be used at a rate faster than the rate of replenishment, and that waste generation should not exceed the carrying capacity of the surrounding ecosystems.

2.1 Characteristics of Sustainability Development

Sustainability is an integration of three issues which are the economic, environmental and social implications. Sustainability of a system is a state reached after it is subjected to SD, where a balance is reached between its economic, environmental and social performance. The SD of a system is measured by the quantification of certain metrics and indicators. These quantifiers are referred to as SD indicators and are derived from a number of quantifying methodologies like Cost-Benefit Analysis (CBA), Environmental Impact Assessment (EIA) and Risk Assessment Matrix.

Since sustainability is a property of the entire system, incorporating sustainability into engineering requires the boundaries of the process to be global expanding beyond the plant. Moreover the scope of the analysis needs to expand beyond economic and performance issues to include environmental, safety and social issues. Hence due to the existence of multiple criteria, a systematic decision making framework is essential for performing a complete and accurate SD of a chemical system. Due to the complexity and multi-disciplinary nature of SD, it can be classified as a Multi-Criteria Decision Making (MCDM) problem.

2.2 Application of SD to Engineering

Every engineering process has an impact on the environment, economy, society and safety of the surroundings, an optimal balance has to be achieved between all these implications to ensure a SD of the process. Hence while designing a process, these impacts have to be identified and optimized by applying either an end of pipe design, redesign or SD. The end of pipe solution is used in all kinds of process industries to meet the requirements of environmental and social constraints, but it does not result in a fundamental change of processing and results in a decrease in the optimality of the existing process design with possible alterations to its productivity and safety features. In most cases the end of pipe designs results in being an obstruction towards long term innovations. Recently redesigning of processes has been applied as a solution to reduction of negative impacts, though this methodology is more effective than end of pipe alterations, it still does not modify the inherent sustainability of a process. Hence in order to ensure a high degree of effectiveness in reducing the negative implications of a process a broader concept of designing the process is necessary and the most suitable methodology for addressing this issue is SD, as it aims to strike a balance between various impacts the process has on the environment, economy, society and safety while satisfying the requirements of all the generations of decision makers.

Figure 1 describes the effectiveness of sustainability development in optimizing the negative impacts of a process in comparison to other methodologies like end of pipe designs or retrofitting.

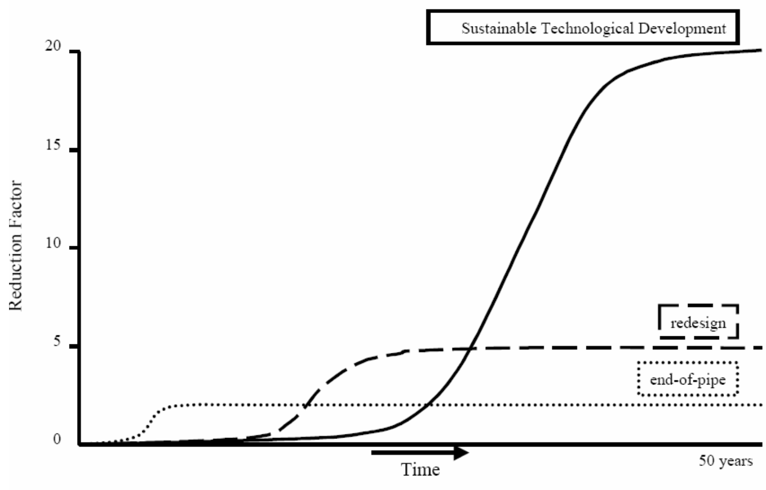

Figure 1 . Time Perspective of Several Solutions for Impact Reduction Factor (Korevaar., Harmsen. Et al., 2000)

3 PROPOSED METHODOLOGY

Any problem solving technique consists of four stages. The first stage is *problem definition* which covers the goals, constraints and the domain knowledge. Following this is the *synthesis* stage where solutions are developed for the problem based on available knowledge and data. The next is the *analysis stage* where the proposed solutions are tested for their applicability and robustness and the most suitable solution is identified. The final stage is the *assessment phase* where the identified solution to the problem is evaluated for its accuracy in satisfying the defined goals within the proposed constraints.

Just like any other problem solving methodology, SD of a chemical process follows the above described four steps.

This research work proposes a decision making framework to identify the most sustainable design for a given chemical process from a set of alternatives. A number of decision making techniques have been used and customized to suit the problem under considerations. Other than these, certain SD indicators and safety indices have been incorporated to quantify the overall performance of the alternatives.

3.1 Proposed Methodology

The proposed decision framework consists of three major steps. Each of these three steps consists of a number of intermediate stages where certain analytical calculations and quantifications are performed. The three steps of the SD decision making framework are as follows:

1. System definition and alternatives identification
2. SD indicators /impact assessment
3. Alternatives comparison and SD decision making

3.2 System Definition

The first step in the proposed methodology is the *system definition* step which aims at defining the boundaries of the system and identifying the subsystems within the existing system. To enable a complete cradle to grave SD, a Life Cycle Analysis (LCA) of the system under consideration is performed. Slight modifications have been done to the process in order to customize it for the problem of SD. Once the system boundary has been established, the succeeding step is to divide the system into a number of subsystems to make the decision making process more robust. The main criterion for identifying the subsystems is to determine the decisions that need to be taken at each stage within the chemical process under development. This step is process dependent and has to be performed for each process for which the decision framework is being used to do sustainability development. This step of *system definition* is analogous to the *problem definition* step of chemical process design methodology.

3.3 Alternatives Identification

Once the system boundary and the subsystems have been identified, the next step is to recognize all the decisions that need to be made regarding the most sustainable process method or design for each subsystem. In order to proceed with this step, all practicable alternatives must be identified for each process or object under consideration. These alternatives were identified by performing literature survey on various studies performed on biodiesel production.

The alternatives identified have been proven to be practicable though not sustainable, hence the main objective of the framework is to identify the most sustainable option from a list of practicable alternatives within each subsystem. This is similar to the *synthesis step* of chemical process designing.

3.4 Impact Assessment Step

Once the alternatives have been identified, in order to do the comparison to identify the most sustainable option, the implication of each alternative on the economy, environment, society and safety must be quantified. This quantification is done by the calculation of certain SD indicators, safety indices and by performing a cost benefit analysis.

For each subsystem, a set of indicators are identified, most of the indicators are common to all subsystems, except for a few case-specific quantifiers or indicators, which vary from one subsystem to the other.

3.5 Decision Making for SD

The final step is the *decision making*, where the most sustainable alternative is identified for each subsystem based on previously defined SD criteria which includes economic, environmental and social feasibility and other performance and safety criteria. Several analytical decision making techniques were studied and finally Analytical Hierarchical Process (AHP), which is a multi-criteria decision making method was chosen for decision making. This method was subjected to minor modification to customize it to meet the requirements of SD. The following sections describe in detail the stages and calculations involved in each of these three steps.

4 SYSTEM DEFINITION – LIFE CYCLE ASSESSMENT (LCA)

LCA is a SD tool that enables quantification of the impact a process has on the economy, environment, society and safety over its entire lifecycle. Although it has been used in a number of industries for about 20 years, more academic and research interest has been shown in this field only since the beginning of the 1990s when its relevance as an environmental management aid in both corporate and public decision making became more evident. Examples of this include incorporation of LCA within the ISO 14000 Environmental Management Systems (EMS), EU Eco-Management Audit Schemes (EMAS), and EC Directive on Integrated Pollution Prevention and Control (IPPC) which require companies to have a full knowledge of the environmental, social and economic implications of their actions both on and off site.

Integration of LCA into SD enables a more global approach to the entire decision making process. LCA is being used widely as a decision making tool and a lot of research is being conducted to constantly improve the process.

In this research work, LCA is used to define the system boundaries. The procedure for incorporating this methodology into the decision making process are reviewed and discussed in the following sections. It is shown that LCA can provide a potentially powerful decision making tool for the management, process engineers and designers.

4.1 Literature Review

LCA has been defined in the previous section as a methodology for assessing the impact a process has on the environment, economy, and society over its entire life cycle i.e. from extraction of raw material to final disposal.

Over the past 20 to 30 years, LCA has been in a process of persistent development and standardization. It is recognized that there is no one way to do the LCA, any methodology is valid as long as it is helpful for understanding and evaluating the magnitude and significance of the potential impacts of a process system (Hoffmann, 2002).

The actual concept of LCA originated from the *Net Energy Analysis* studies, which were first published in the 1970's and considered only energy consumption over a life cycle of a process, some later studies included wastes and emissions**,** but none of them went further than just quantifying materials and energy use. Further improvements were required in the developed methodologies to approach more complex processes which had a wider area of impact.

In the early 1990s the Society for Environmental Toxicology and Chemistry (SETAC) were actively involved in developing a robust methodology for performing LCA on complex chemical processes. Soon, the International Organization for Standardization (ISO) started similar work in developing principles and guidelines on the LCA methodology. Though the two organizations, ISO and SETAC, conducted research separately, a general consensus on the LCA framework between the two started to emerge with minor differences in the matter of detail. While the ISO methodology is still being modified, the methodology developed by SETAC is more widely used by LCA practitioners.

Many well known LCA derived approaches such as the Eco-Indicator (Goedkoop and Spriensma, 2000) and Eco-Efficiency (Saling, 2002) have been used extensively in process development. Recently application of LCA in SD has emerged with a number of researchers are actively involved in developing SD frameworks incorporating LCA into them.

4.2 Life Cycle Assessment and SD

In theory, LCA made a suitable analysis tool for environmental impact assessment of complex processes, but due to its well developed framework and already wide application, it can be customized to assess the economical as well as social implications of complex processes. The only bottleneck lies in incorporating the SD indicators into the entire process.

The actual process of life cycle assessment consists of four steps; 1) scope and goal definition, 2) inventory analysis 3) impact assessment and 4) interpretation. The third step impact assessment aims to convert the economic, social, environmental and safety implications of the process into SD indicators that can be used as metrics for evaluating and comparing available alternatives. Most of these SD indicators are unit less quantities or are expressed as financial loads that can be compared on a pair wise basis.

4.3 Framework for LCA

LCA follows the life cycle of a product or a process from extraction of raw materials to final disposal, including manufacturing, transportation, use, re-use, maintenance and recycling (Azapagic, 1999), this is illustrated in Figure 2. Its main advantage over other, site specific methods for SD lies in broadening the system boundaries to include all the implications a process has and not just focusing on the impact felt in the processing or manufacturing stage.

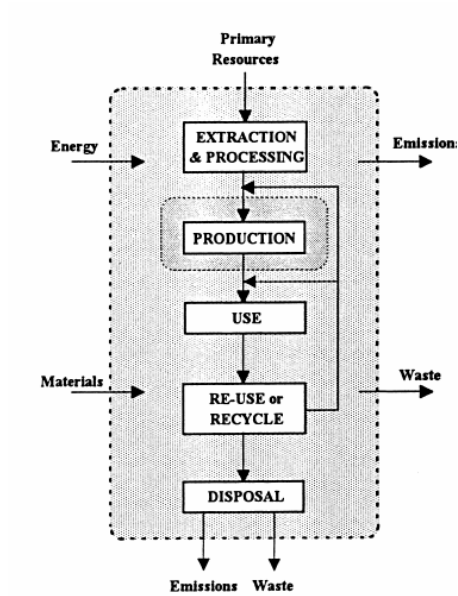

Figure 2 . LCA System Definition (Azapagic, 1999)

LCA is based on a thermodynamic and system analysis, which are central to process engineering (Azapagic, 1999). The first step is the identification of the boundaries and hence the definition of the system under review for SD.

4.4 Goal Definition and Scoping

The boundary identification of a system in the LCA should be made as global as possible. The principle factors to be considered are the material and energy flows within the primary process of the system, but in addition to these, sub processes involved in the extraction or manufacturing of the raw materials and production of intermediate feedstock must be included. Intermediate feedstock can be defined as ancillary materials that are used indirectly in the production of the final product, like for example the fertilizers used in the growth of the biomass feedstock. Means of disposal of products, by-products, excess reactants and wastes should also be included within the LCA system boundary. The system concept shown in Figure 3 clearly illustrates the meaning of the terms, boundary, process, intermediate feedstock and materials.

It is important to assign the extent to which the boundaries should extend upstream of the process. In most scenarios the impacts of upstream processes become less significant the further they are away from the main process, and a situation of diminishing returns becomes apparent past the third level of upstream processes. The determination of the system boundaries is based on data availability.

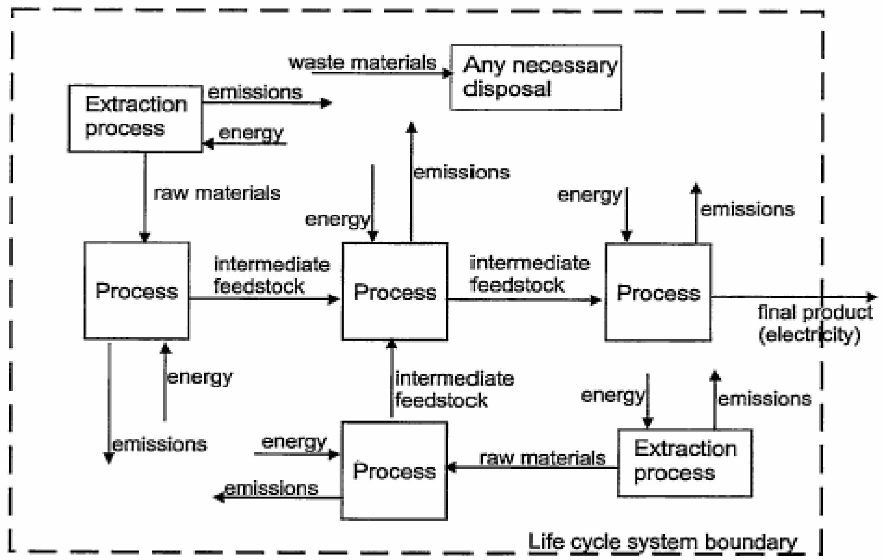

Figure 3 . System Concept in LCA (Mann. and Spath., 1997)

For this particular case study of bio-diesel production, data on extraction of raw materials, processing, manufacturing, and delivery to point of use for most process feedstock such as the biomaterials, fertilizers used for the growth of these biomass feedstock, chemical reactants and fuel used in the process was available hence these were included within the system boundary. Thus the system included nearly all of the major processes required to produce bio-diesel from biomass. Certain operations such as the construction of the facilities to manufacture the transportation equipment, and manufacture of harvest hardware were felt too far from the scope of the system and of diminishing significance in comparison to the other operations and hence were not included within the system boundary.

4.5 Inventory Analysis

Life Cycle Inventory Analysis (LCIA) is a method for estimating the consumption of resources and the quantities of wastes flows and emission caused by or otherwise attributable to a process/product life cycle (Azapagic, 1999). The processes within the lifecycle and the associated material and energy flows as well as other exchanges are modeled to represent the product system and its total inputs and outputs from and to the natural environment, respectively. These results in a product system model and an inventory of environmental, economic and social implications related to the system under review. The first step in this analysis is the identification of sub-systems within the larger system. In this study the subsystems identified are the raw materials (biomass, reactants and catalysts), process types (overall process type, glycerol extraction method, bio-diesel purification method), end product usage (bio-diesel mixture ratio and byproducts usage). The subsystems identified for the bio-diesel case study are shown in Figure 4. For each of these subsystems alternatives are identified from research work conducted on bio-diesel (Zhang, Dube et al., 2003) (Tapasvi, Wiesenborn et al., 2005) (Rudolph and He, 2004) (Roszkowski, 2003) (Demirbas and Karslioglu, 2007) (Besnainou and Sheehan, 1997). The identified alternatives have been proven to be practicable though not sustainable; hence the main objective of the framework is to identify the most sustainable option from a list of practicable alternatives within each subsystem. The alternatives identified for each subsystem are illustrated in Table 1.

Table 1

Bio-diesel Subsystem Alternatives

Subsystem	Alternatives
Bio mass	Soy Bean
	Rape Seed Oil
	Sunflower Oil
	Beef Tallow
Catalyst	Basic
	Acidic
	Enzymatic
Alcohol	Methanol
	Ethanol
Production Process	Thermal Cracking
	Transesterification
Glycerol Extraction	Gravitational Settling
	Centrifuging
Bio-diesel Purification	Hexane Extraction
	Water Washing
Bio-diesel Mix Ratio	Direct Use
	Blending

The main objective of the LCIA is to quantify the resources requirement and waste and emission generation with respect to each sub-system. Each process system is usually a static simulation model composed of unit processes, which each represent one or several activities such as production processes, transport or retail. For each such unit process, data are recorded on the inputs of natural resources, emissions, waste flows, expenditures, safety issues, social implications and other environmental impacts. The environmental and economic implications are assumed to be linearly related to one of the product flows of the unit process.

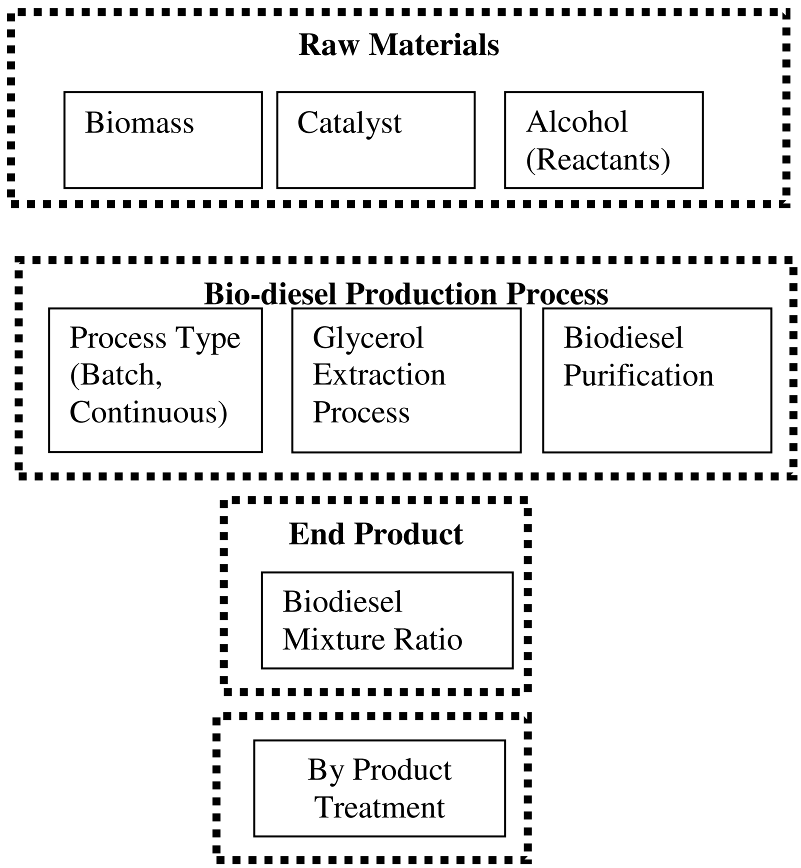

Figure 4 . Bio-Diesel Subsystem Alternatives

5 IMPACT ASSESSMENT – SD INDICATORS

The most important part of LCA with respect to SD is the impact assessment step. According to ISO 14042, impact assessment can be performed in a sequence of steps: a) defining impact categories, b) identifying category indicators, c) selection of characterization models, d) classification, f) normalizations, g) grouping and h) weighing.

The first three steps are the most important as they define the metric to be quantified. But due to lack of professional knowledge requisite and limited availability of data, these steps are performed in a rather pre-devised pattern with little controllability left to the user.

The description of these SD indicators is discussed in the SD section. These indicators are divided into four categories, 1) Environmental; 2) Economic; 3) Safety; 4) Social. In this research work the first four indicators are analyzed and applied in the SD of bio-diesel production.

Another important step in impact assessment is aggregation of the various indicators into subgroups and attaching weights to the impacts to indicate their relative importance. The method chosen in this research work to do it is by AHP. This step is the most controversial part of the LCA as it implies subjective value judgments in deciding the importance of different impacts. The scales used for the hierarchical arrangement of the impacts are mostly decided upon by the decision maker, experts in that particular field of study or by the public.

5.1 Identifying Impact Categories - SD Indicators

The first step in impact assessment is identifying the impact categories and the category indicators. The quantification of these implications is done by the evaluation of SD indicators and safety indices. SD indicators quantify the environmental, economic, social and safety implications of a process and their life cycles to facilitate sound decision making. The challenges in developing such indicators for industrial processes and the variety of existing approaches are described in recent papers. Popular approaches relevant to chemical processes include those developed by the American Institute of Chemical Engineers in the United States and by the Institution of Chemical Engineers in the United Kingdom. Similar efforts are also being made by industry groups such as the Global Reporting Initiative and the World Business Council for Sustainable Development. Due to these efforts, a number of practical and industrially relevant metrics have been developed and applied to quantify the SD of processes. These indicators include measures of environmental impact in terms of pollutant release, land, water and resource usage; process performance in terms of productivity, and direct and indirect implications of the process on safety, economy and the society. Use of the SD indicators follows the simple rule that the lower the metric the more effective the process. A lower metric indicates that the impact of the process is less and the output of the process is more. Despite the lack of a rigorous theory or definition, many SD indicators have been developed. These indicators should be easy to calculate with available data, useful for decision making, reproducible, scientifically rigorous, useable at multiple scales of analysis, and extendable with improves understanding. The concept of SD often requires macro scale consideration of the environment, economy and society, despite the fact that the actual decisions are made at a finer scale. Thus there is a need for methods that can translate the impact of the decisions made at a micro scale on to a larger more global scale, and, conversely interpret global sustainability goals and indicators to enable detailed decision making at a micro scale. This requires the SD indicators to be hierarchical or nested to permit communication between different levels of an organization. Aggregated indicators are sufficient for management decision making, but detailed metrics and indicators are essential for process optimization and improvement. There is a constant need for improvement in the handling of the uncertainties in the metrics and the potential interactions and redundancy between multiple metrics representing different goals. Multivariate statistical methods like those used in process monitoring may be useful. As new sustainability quantifying methods are being developed to aggregate and balance the various requirements of SD of a process, companies are required to modify and refine their decision making methodology to ensure maintenance of process sustainability.

The SD indicators are quantifiers of the economic, environmental, safety and certain other impacts of a system all through its life cycle. A detailed description of each of these indicators is given in the later subsections of this section. Other than the usual economic, environmental and social indicators, certain other impact quantifiers can be used as SD indicators such as safety indices, fuel performance factors and productivity indicators depending on the system under review. Some of these indicators along with the commonly used SD indicators are displayed in Table 2.

Table 2

Basic SD Indicators

Implication	Indicator
Economic	Total Capital Costs
	Total Manufacturing Costs
	After Tax rate of return
	Break Even Price
Environmental	Environmental Performance Indicators
	Land Usage
	Water Usage
Fuel Performance	Cetane Number
	Carbon %
Safety Indicator	Risk Assessment Matrix
	Inherent Safety Indicators
	Flash Point
	Inherent Safety Indicators
Raw Material Indicators	Fuel Purity
	Bio-diesel Yield

5.1.1 Economic Indicators

Economic indicators are based on expenses and financial returns associated with the process. The economic indicators in general should quantify hidden costs associated with the utilization of raw materials, energy, capital and human resources; as well as estimate uncertain future costs associated with external impacts of the industrial activity; address full costs and benefits incurred by various stakeholders across the life cycle of the process and value the impact the process has on natural and social capital. Valuation techniques that convert all costs and impacts into monetary terms are the most attractive but these are highly subjective and lack a sound ecological or physical basis.

In this research work, two major economic indicators are used to quantify the economic implications of the process. The economic indicators used mainly are based on the principle of cost benefit analysis. The economic indicators used are shown in Table 3. The economic performance of a process is quantified by determining the capital cost, manufacturing cost and the break even price. The economic indicators are determined once certain parameters such as the plant capacity, process technology, raw material and chemical costs are determined. These indicators can also be used as comparison parameters to select from a list of alternatives the most sustainable one. The first economic indicator to be discussed is the capital cost, according to the definition of capital cost estimation (Turton, Bailie et al., 1998) it includes three parts, the total bare module capital cost, contingencies and costs associated with auxiliary facilities. Total bare module capital cost is the sum of the cost of each piece of equipment in the process. Contingencies and fees are defined as a fraction of the total bare module capital cost to cover unforeseen circumstances and contractor fees (Turton, Bailie et al., 1998). Expenses of auxiliary facilities include items such as purchase of land, installation of electric and water systems and construction of internal roads. They are represented by 30% of the total basic module cost. Total capital investment is calculated by adding the fixed capital cost to the working capital cost. The latter is usually a fraction of the fixed capital cost.

Total manufacturing cost refers to the cost of the day-to-day operations of a chemical plant and is usually divided into three categories: direct manufacturing costs, indirect manufacturing costs and general expenses. After tax rate of return is a general economic performance criterion for the preliminary evaluation of a process plant and is defined as the percentage of the net annual profit after taxes relative to the total capital investment. Net annual profit after taxes is equal to income after taxes and is half of the net annual profit when a 50% corporate tax rate is used (Ulrich, 1984). After-tax rate of return was also chosen as the response variable and the objective function in the economic assessment in this research work. Break even price is defined as the price for which revenue from biodiesel product is the same as total manufacturing cost of a plant. The break even price has been quoted as an economic parameter in previous publications (Zhang, Dube et al., 2003). These parameters are used as comparison parameters for identifying the most economically sustainable option from a set of alternatives.

Table 3

Economic Indicators

Type	Indicator	Description
Costs	Total Capital Costs	Total Bare Module Costs + Contingencies + Auxiliary Facilities Cost
		Fixed Capital + Working Capital Costs
	Total Manufacturing Costs	Direct + Indirect Manufacturing Expenses
Returns	After Tax Rate of Return	% of Net Annual Profit after taxes relative to Total Capital Costs
	Break Even Price	Price of Bio-diesel for which Revenue from Bio-diesel = Total Manufacturing Costs

5.1.2 Environmental Indicators

In most cases environmental impact indicators are measurements of annual emissions of chemical components such as $C0_2$, NO_x, VOC, SO_x emissions. But these measurements have certain disadvantages as they are negligent of the net impact on the environment, as these various chemicals are not all equally toxic nor do they affect the environment to the same extent. In order to overcome these disadvantages, authorities, industries and other stakeholders have been trying to establish a link between the reported emissions per chemical component and the actual environmental impacts. A result of research in this field has resulted in the development of the Environmental Performance Indicator (EPI) method (VNCI., 1999).

This method defines seven environmental effects: global warming, eco toxicity etc. For each environmental effect one single EPI is defined numerically represents the extent of the impact of that particular component on the environment. There are in total seven indicators that represent numerous environmental effects of a number of chemical components. The calculations associated with EPI are simple, transparent, easily auditable and similar for all indicators. Within each environmental effect, the associated EPIs can be aggregated to represent the total impact of a particular process. The individual contribution per chemical component is also identifiable in this methodology for each process. In the current methodology only the emission to air and surface water are considered.The required measurements to determine the EPIs are the measurement of emissions to air and surface water, on a chemical component basis, expressed in kg/year. The EPI – method groups the impacts of emissions into the atmosphere and/or into surface water into seven categories as shown in Table 4. The first column refers to the type of the environmental effect and in total there are seven effects addressed in this methodology of environmental impact assessment. The second column refers to the unit used to quantify the effect with respect to the chemical under study. The third column gives the name of the EPI used while displaying the results of the calculations and finally the last column refers to the chemical which is used as the base case for that particular environmental effect. The environmental impact of other chemicals is compared to the environmental impact of the reference chemical and their EPI is expressed in terms of equivalent weight of the reference chemical.

Table 4

Environmental Performance Indicators by Environmental Effect

Environmental Effect	**Expressed in terms of**	**EPI Name**	**Reference Chemical**
Global Warming	Heat Radiation Absorption Capacity	Global Warming Potential (GWP)	CO2
Depletion of Ozone Layer	Ozone depletion capacity	Ozone depletion Potential (ODP)	CFC -11
Photochemical Ozone Creation	The change in ozone concentration due to a change in the emission concentration of a chemical	Photochemical Ozone Creation Potential (POCP)	Ethylene
Acidification	Acidifying effect on the ecosystem	Acidification Potential (AP)	SO2
Human Toxicity	Toxicity to humans	Human Toxicity Potential (HTP)	1,4 -Dichloro Benzne
Eco Toxicity	Toxicity to aquatic ecosystem	Eco Toxicity Potential (ETP)	1,4 -Dichloro Benzne
Eutrophication	Contribution to the creation of biomass	Eutrophication Potential	Phosphate

The basic principle of the method is to calculate a performance indicator with respect to each chemical component emitted. Each EPI is calculated by multiplying all the individually identified chemical component emission (in kg/year) with a unique "*Weighing Factor*" and by finding the aggregate of all the weighted results within the associated effect category. The weighing factors used are unique per component, per impact category, and per destination of the emission (air or surface water). The illustration below gives the step by step procedure to calculate the EPI for a particular process:

Step 1: The starting point is the (annual) list of emissions per chemical component into water and/or into the atmosphere, expressed in terms of kg/year.

Step 2: For each individual chemical component emission, the '*Unique Weight Factor'* is determined. This is done for all the emissions both into water and into the atmosphere. A single chemical can contribute to more than one environmental effect; in such cases the list of '*Unique Weight Factors'* will list as many values

Step 3: The emissions are arranged according to the appropriate environmental effect. A single emission can be classified under more than one category. Distinction between emissions into water and emissions into the atmosphere (important for Human Toxicity, Eco Toxicity and Eutrophication) is made.

Step 4: For each chemical component the contribution to the relevant EPI using the formula:

$$C_i = \sum e_i \text{ x } WF_{ji}$$

Where,

C_i = Contribution to the relevant EPI by chemical i

e_i = emission of chemical i in kg/year

WF_{ji} = Weighing factor for chemical i for the environmental impact j

Step 5: Aggregate of all the individual environmental contributions is calculated to arrive at the total EPI value. This is to be repeated for all the categories

Step 6: For each environmental effect a group of chemical components is determined for emissions into both water and the atmosphere. Certain chemicals may contribute to various effects and will have different weight factors, one for each effect. An example calculation is shown in Figure 5.

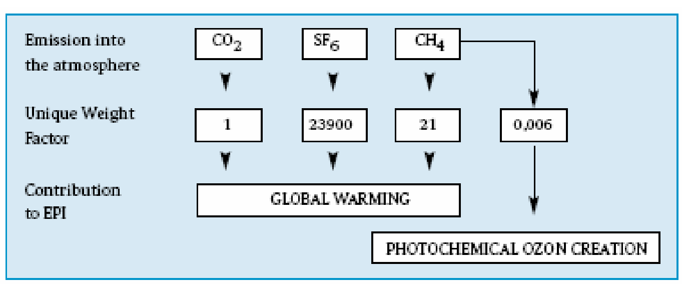

Figure 5 EPI Calculation Example

In this example shown above, three well known green house gases: CO_2, SF_6 and CH_4 are considered. The reference chemical for global warming is $C0_2$ hence it is given a weighing factor of 1. This means that other chemicals have been compared to 1kg of CO_2 for assessing their relative global warming effect. The unique weighing factor for CH_4 is 21, which means that 1 kg of methane contributes 21 times more to global warming than 1 kg of $C0_2$. The unique weighing factors for about 250 chemical components are available.

Other than the Environmental Performance Indicators (EPI), other quantities are also used for measuring the environmental impact for this particular system of biodiesel production. As the end product is bio-diesel, certain fuel working properties are also used to assess the impact of the fuel on the environment. A brief description of the fuel properties used for comparing different bio fuel feed-stock is listed in Table 5.

Table 5

Environmental Impact Indicators for Bio-Diesel System

Type	Indicator	Description
Environmental Impact	Environmental Performance Indicators (EPI)	Σ (Emission (kg/yr) * Unique Weight Factor)
Fuel Performance Indicator	Cetane number	Measure of aromatic content, Fuel ignition characteristics
	Carbon %	Measure of carbon in fuel

5.1.3 Safety Indicators

Though safety has not been considered an integral part of SD, it has been proven over the period of time that safety directly as well as indirectly affects the economics and performance of any chemical process system. Hence it is important to make safety and integral part of SD. Safety is a concept covering hazard identification, risk assessment and accident prevention (Kharbanda and Stallworthy., 1988).

There are a number of ways to measure the safety implications associated with a system, one of the best known measures is the risk estimation. Risk can be defined as the mathematical probability of a specified undesired even occurring, in specified circumstances or within a specified period of time. In a chemical process such losses may be damage to equipment, loss of production, environmental damage or an injury or death of personnel (Taylor, 1994). Risk involves two measurable parameters: consequence and probability. Some events are more likely to occur than others, but a unique consequence of the sequence of events cannot be predicted (Heikkilae, 1999). Another important term that needs to be discussed while addressing safety is hazard which can be defined as a condition with the potential of causing an injury or damage. A number of hazards can be associated to a chemical process over its lifetime such as the toxicity or reactivity of the raw materials and chemical reactants involved, energy releases from the associated chemical reactions, extreme temperature and pressure conditions, quantity and toxicity of intermediates involved etc.. Each of these hazards impacts the overall process risk. The best method to identify the degree of risk involved in a process is by employing a Risk Assessment Matrix (RAM). RAM has been used in the chemical industry to rank different risks in order of their severity for prioritizing the implementation of control measures. The main feature of a RAM is the inclusion of the two variables, probability and consequence. These two variables can be represented in the matrix in either a qualitative terms or in quantitative values, in this research work, a combination of both these methods is employed. In a typical RAM, there is a step-wise scaling of the severity of the consequences represented as rows and a step-wise scaling of the probability of occurrence of a particular hazardous event represented as the columns. The severity of any risk is quantified based on their position in the matrix which directly depends on the severity of their consequence and the frequency of occurrence.

The basic steps involved in using a RAM are as follows:

1. Selection of targets: These can be illness/injury/health of personnel, equipment productivity (downtime), equipment loss, product loss, environmental damage and monetary penalty.
2. Definition of the probability and severity scales for each target
3. Hazard identification: Listing of all possible and significant hazards associated with each subsystem.
4. Establishment of the Risk Tolerance Levels: Depending on the severity of the consequence and the probability of occurrence the regions within the matrix are divided into High, Medium and Low Risks.

5. Risk Assessment: For each identified hazard within every subsystem, the associated risk is classified into the Low, Medium or High risk category.

The targets identified for the case study of biodiesel in this research study are the injury/health effects on personnel, environmental effect of the event, asset damage and other monetary implications and impact on reputation.Table 6 illustrates the RAM used in this research work for assessing the risks associated with each subsystem within the biodiesel system under review.

Table 6

Risk Assessment Matrix

Severity of Consequences	Probability of Occurrence				
	A	B	C	D	E
Negligible 0		**LOW**			
Minimal 1					
Marginal 2			**MEDIUM**		
Critical 3				**HIGH**	
Catastrophic 4					

For each of the targets identified above, the severity and the probabilities need to be interpreted. The consequence estimates are based on envisaged scenarios of what "might happen" and the probability estimates are based on historical information that such a scenario has happened under similar conditions, knowing full well that circumstances can never be exactly the same. For consequences a scale of 0 to 4 is used to indicate increasing severity. The probabilities are listed as A to E with increasing likelihood of occurrence and these probabilities refer to the likelihood of the occurrence of the estimated consequence and not the likelihood that the hazard is released. Like for example, a hazard has been identified to occur several times in a year and create a situation with a number of fatalities. However, in the history of the process under review, it has never resulted in a fatality, so instead of assigning a lower likelihood it has to be assigned a higher likelihood of occurrence. Tables 7 through 9 define the levels of the severity of consequence to personnel impact, environmental effect, and asset damage / monetary implications, respectively.

Table 7

Personnel Impact

Level	Description
0	No injury or damage to health
1	Minor Injury/health effects – Lost time injury inclusive of restricted work case or occupational illness and lost workday case
2	Major injury/health effects - Permanent partial disability and occupational illness
3	Permanent total disability or one to three fatalities
4	Multiple fatalities from an accident or occupational illness

Table 8

Environmental Impact

Level	Description
0	No damage or financial consequences
1	Slight damage within the system's physical boundaries, negligible financial consequences
2	Localized effect - limited discharges affecting neighborhood and repeated violation of statutory limits and multiple complaints
3	Major Effect - Severe damage with widespread impact, requiring extensive restoration measures. Extended violation of statutory limits.
4	Massive Effects - Persistent severe damage extending over large areas along with severe financial consequences.

Table 9

Asset Damage / Monetary Implications

Level	Description
0	Zero damage
1	Brief disruption (Damages <1 $10,000)
2	Partial Shutdown but can be restarted (Damages up to $ 50.000)
3	Partial operation loss (Damages up to $100,000)
4	Substantial or total loss of operation (Damages up to $ 1 Million)

Unlike the severity levels the probability of occurrence definition for the letters A – E is the same for all the targets. The description of these letters is given in Table 10. The definition used in this research work is quantitative for probabilities and qualitative for the consequence severities. This makes the RAM partially qualitative and quantitative.

Table 10

Probability Scale

Letter	Description
A	Negligible
B	Once in more than 10 yrs
C	Once every 1 to 10 years
D	Once every 6 months to 1 year
E	Once every < 6 months

Hence in this research work the major SD indicators evaluated for each of the alternatives are the economic, environmental, safety and certain system specific impact quantifiers. These SD indicators are used to calculate the parameters used in the comparison of the various alternatives. The AHP pair-wise comparison scoring scales are based on these comparison parameters and have been explicitly defined for each subsystem for each SD indicator. The next section describes the proposed methodology for the decision framework for SD of a process or product.

6 DECISION MAKING FOR SUSTAINABILITY DEVELOPMENT

Decision making for SD of a chemical process can be considered as a multi criteria decision making (MCDM) process. MCDM is applicable to SD due to the multi field nature of sustainability. SD considers the impact a process has on the economy, environment, society and safety and the requirements of a current generation of stake holders as well as the needs of future generations of stake holders. This wide region of impact of SD of a process makes it a problem with multiple criteria to be satisfied. Some of the commonly used MCDM techniques are the AHP, distance function method and the Multi Attribute Utility Theory (MAUT). Of the three techniques, AHP is the most suitable for decision making for SD as it best handles multiple criteria and alternatives. The AHP is characterized by three principle functions: 1) hierarchical structuring of complexity; 2) ratio scale measurement derived from pair-wise comparison; and 3) synthesis of priorities (Forman and Gass, 2001; Saaty, 1987; Saaty, 1994). The outcome of an AHP is a prioritized ranking or weighing of each decision alternative. The ranking scale applied in AHP, as shown in Table 11, is used for prioritization of the SD indicators as well as for the comparison and prioritization of the alternatives with respect to each SD indicator.

The following are the calculation involved in this comparison process:

1. Identify the alternatives to be prioritized in each subsystem.

2. Determine the SD indicators that are used in the selection of the most sustainable alternative within each subsystem.

3. Define the comparing scale for prioritizing the SD indicators. In this step a comparison scale is defined for the SD indicators identifying their degree of impact. There are three degrees of impact: low, medium and high. Figure 6 illustrates the definition of these degrees of impact for the environmental, social and economic implications.

Environmental	Economic	Social
Zero	No Diff	No Impact
Slight Effect/No financial consequences	<10% Total Investment	Slight Impact
Minor Damage/ <$1K to correct and/or in penalties	10-25% Total Investment	Local regional Impact
Short Term (<1 yr) damage/ $1K - $250K to correct and/or in penalties	25-50% of Total Investment	National level impact
Medium Term(1-5yrs)/$250K-$1M to correct and/or in penalties	50-75% Total Investment	Global Impact
Long Term(>5yrs)/ > $1M to correct and/or in penalties	**75-100% of Total Investment**	**--------------------**

Figure 6 Degrees of Impact for the SD Indicators

In Figure 6 situations are defined classifying the degree of impact of each implication into three categories of high, medium and low. Corresponding number scores are allotted to the SD indicators depending on their degree of impact to be used while performing the pair-wise comparison in AHP. Table 11 illustrates the color legend for the SD indicator priority table and the corresponding numerical scores. The scoring scale varies from 1 to 3, with 1 representing equal impact or performance, 2 representing moderate difference and 3 signifies well marked difference between the two alternatives with one being strongly preferred over the other. The indicator with the higher level of priority is given the higher score and the other indicator is given the reciprocal of the score. For example if one indicator is assigned medium priority and is compared with an indicator assigned a low priority then the medium priority indicator gets a score of 2 and the low priority indicator gets a score of 0.5. The scaling used is qualitative for all the three SD indicators and based on historic data and expert opinion.

Table 11

Priority Scoring for SD Indicators

LEVEL	SCORE
HIGH	3
MEDIUM	2
LOW	1

AHP SCORE	DEFINITION- Diff in level of impact
1	Same
2 or 0.5	1 Level
3 or o.33	2 Levels

Once the priorities have been assigned to the different SD indicators, the next step is to perform the AHP comparison to determine the relative priority scores. For the safety indicators, the level of importance is based on the risk index obtained for that particular subsystem from the RAM discussed in the previous section. The high risk category is given the maximum score of 3 and the low risk category the minimum score of 1.

4. Define the comparison scale for the alternatives with respect to each SD indicator. Comparison parameters are used to compare alternatives with respect to each SD indicator. These comparison parameters are calculated from the SD indicators evaluated for each alternative. As these comparison parameters vary in both units and magnitude from one SD indicator to another the AHP scale used also varies from one indicator to another. Tables 12 through 17 illustrate the AHP scales used to compare the alternatives with respect to environmental, economic and safety implications. For certain sub-systems, other than the above mentioned three SD indicators certain system specific indicators like fuel performance indicators or yield percentage, purity etc are evaluated.

Table 12

Environmental Indicators

% Diff in EPI, Land Usage, Water Usage	AHP Score
-65	3
-15	2
0	1
15	0.5
65	0.33

Table 13

Fuel Performance Indicators

Diff in Carbon %	AHP Score
-65	3
-15	2
0	1
15	0.5
65	0.33

Table 14
Raw Material Indicator

% Diff in Fuel Purity, Bio-diesel Yield	AHP Score
65	3
15	2
0	1
-15	0.5
-65	0.33

Table 15

Economic Indicator

% Diff in Total Capital Costs, Manufacturing Costs	AHP Score
-500	3.00
-25	2.00
0	1.00
25	0.50
500	0.33

% Diff in Break Even Price	AHP Score
-50	3
-25	2
0	1
25	0.5
50	0.33

Table 16

Safety Indicator

Risk Index	Number Score
High	3
Medium	2
Low	1
Diff in Risk Index	AHP Score
-2	3
-1	2
0	1
1	0.5
2	0.33

% Diff in Flash Point	AHP Score
65	3
15	2
0	1
-15	0.5
-65	0.33

5. Construct an N × N matrix to prioritize N SD indicators. Use the scale defined to allot the scores (1/2/3) for each pair-wise comparison. The proposed method makes use of pair-wise comparison of the alternatives and assigning scores with respect to each comparison parameter using a comparison scale specific to that particular parameter. The scale used for this pair-wise comparison is shown in Table 11 and the methodology of allotting these scores are explained in detain in the AHP section.

6. Normalize the scores obtained by dividing each cell with the sum of all the other cells in the same column as the cell.

7. Final score for each indicator is obtained by averaging the normalized score in all the cells in the same row as the indicator.

8. The above steps are performed to arrive at the priority score for each SD indicator.

9. The predefined scales for the comparison scores for the subsystem alternatives with respect to each SD indicator are used to assign the scores for the alternatives. The scales for the different SD indicators are defined in Tables 12 to 17 in step 4 for this section. A detailed description of the process of AHP for alternatives prioritization is given in step 4 and illustrated with an example in the Case Study section.

10. Final score for each alternative is obtained by averaging the product of the priority score of an alternative for each SD indicator with the corresponding SD indicator priority score.

$$FinalScore = \sum A_i \bullet P_i$$

Where,

A_i = Priority score of Alternative i with respect to SD indicator i

P_i = Priority score of SD indicator i

11. Final selection: For each subsystem the same methodology is utilized to identify the most sustainable alternative. Each alternative for a given subsystem is assigned a priority score with respect to each comparison parameter and each comparison parameter has a priority score with respect to the subsystem under consideration, the two priority scores are used to determine an overall priority score for each alternative. The alternative with the highest score is identified to be the most sustainable as it has an overall better performance with respect to environmental, economical, safety and social implications. Hence the methodology ensures a decision making which follows the principles of SD.

7 CASE STUDY – BIO-DIESEL PROCESS

The proposed methodology for decision making for SD of a process has been applied to the bio-diesel system. The final product of the proposed methodology is a completely sustainable bio-diesel system.

The first step in the proposed methodology is to identify the bio-diesel system to which SD is to be applied. Within this system, subsystems are identified and suitable alternatives for each of these subsystems are subsequently identified and listed. The subsystems and the corresponding alternatives selected using the proposed methodology, are shown in Table 10 in section 5.1.3.

In this section, for each subsystem the prioritization and the quantification of the SD indicators are discussed in detail with supporting tables and visualizations. The reasoning for the prioritization of the alternatives with respect to each of the SD indicators and the method of selection of the most sustainable alternative is also discussed.

7.1 Raw Material Subsystem

The raw material subsystem within the bio-diesel lifecycle system; is the first subsystem subjected to SD using the developed framework. In this case study the raw materials considered are soy-bean, rape seed, sunflower and beef tallow. Since these are widely cultivated, available and economically viable they are the most commonly used feedstock for bio-diesel production. The SD indicators used are environmental indicators (EPI, land usage, water usage); economic indicators (total capital costs, manufacturing costs, after tax rate of return, bio-diesel break even price); safety indicators (RAM index) and certain system specific indicators (fuel Cetane number, fuel carbon %).

7.1.1 Prioritization of SD Indicators

The next step is the prioritization of these indicators based on their degree of importance with respect to that particular subsystem. The scale and scoring key defined in Figure 5 and Table 11 are used in AHP comparison and the priority scores are obtained for the different SD indicators. Table 18 indicates the priority levels assigned to the SD indicators for the raw material subsystem. As raw material is the highest contributor to the bio-diesel price, economic indicators are given the highest priority. Since feed-stock is used in the largest quantity among all the raw materials for bio-diesel production, its impact on the environment must be given high priority when considering the life cycle environmental impact of bio-diesel. Since there are no major safety-issues associated with raw materials manufacturing or use, safety indicators are given medium priority. Certain fuel properties such as cetane number and percentage of carbon depend largely on the raw material used and are hence used as indicators which are given high priority like the environmental and economic indicators. Table 18 also lists the numerical scores corresponding to the priority level for each of the SD indicators.

Table 17

SD Indicator Priority Level Assignment

Indicator	Priority Level	Number Score
Environmental	HIGH	3
Economic	HIGH	3
Safety	MEDIUM	2
Fuel Performance	HIGH	3

The priority levels are given corresponding numeric scores to enable easy calculation in the AHP template as shown in Table 18. Table 19 illustrates the first step in AHP which is the pair-wise comparison and score allocation for the different indicators using the predefined comparison scale. (Table 11).

Table 18

AHP Template for Prioritization of the SD Indicators

Step 1	Environmental	Economic	Safety	Fuel Performance
Environmental	1	1	2	1
Economic	1	1	2	1
Safety	0.5	0.5	1	0.5
Fuel Performance	1	1	2	1

Table 20 illustrates the second step in AHP comparison which involves the neutralization of the pair-wise comparison scores and calculation of the final priority score for each SD indicator with respect to the raw materials subsystem.

Table 19

Final Score Evaluation

Step 2	Environmental	Economic	Safety	Fuel Performance	Priority score
Environmental	0.286	0.286	0.286	0.286	0.286
Economic	0.286	0.286	0.286	0.286	0.286
Safety	0.143	0.143	0.143	0.143	0.143
Fuel Performance	0.286	0.286	0.286	0.286	0.286

7.1.2 Selection of Sustainable Alternative

An AHP template is used to compare the alternatives with respect to each of the SD indicators and prioritize them based on their performance using the pre-defined AHP scoring scales. The first SD indicator used for the comparison of the raw-material alternatives is the environmental indicator, EPI. Table 19 shows the EPI values in terms of CO_2 weight equivalent emission for each raw-material. These values are based on the amount of green house gases emitted during fertilizer manufacturing, cultivation, harvesting and oil recovery as well as the amount of N_2O released during cultivation of the feedstock which is converted into CO_2 weight equivalents (Jungmeier, Hausberger et al., 2003). It was observed that soy-bean required much less fertilizer than both rape seed and sunflower. Rape seed cultivation requires large amounts of nitrogen fertilizers and hence its impact on the environment is higher in comparison to sunflower and soy-bean. Beef tallow was given the highest EPI score since more energy is input into the pre-processing of this raw material to be used as a feedstock for bio-diesel production.

Other than EPI, land and water usage are also used as environmental impact indicators. The land and water usage for the alternatives are qualitatively assessed as high, medium or low and are assigned corresponding numerical scores. Table 21 lists all the environmental indicators for all the raw material alternatives.

Table 20

Environmental Indicators for Raw Materials

Alternatives	Environmental				
		Land Usage		Water Usage	
	EPI	Usage Level	Number Score	Usage Level	Number Score
Soy-bean	40	MEDIUM	2	MEDIUM	2
Rape Seed	110	LOW	1	MEDIUM	2
Sunflower	70	HIGH	3	HIGH	3
Beef Tallow	140	MEDIUM	2	MEDIUM	2

Once the environmental indicators are quantified, the next step is to perform the pair wise comparison of the alternatives using an AHP template, with respect to each of these indicators and obtain individual performance scores. The first step of this comparison is shown in Table 22; the scores are assigned based on the scale defined in Table 12 for environmental indicators. Then the next step of AHP which is the normalization of these pair wise comparison scores and the calculation of the final indicator score for each of the raw material alternative is shown in Table 23. These steps are repeated for obtaining the individual indicator score for all the three environmental indicators for all the alternatives.

Table 21

AHP Template for Prioritization of Raw Materials with Respect to EPI

STEP 1	Soy- Bean	Rape Seed	Sunflower	Beef Tallow
Soy-Bean	1	3	3	3
Rape Seed	0.33	1	0.5	3
Sunflower	0.33	2	1	3
Beef Tallow	0.33	0.33	0.33	1

Table 22

Final Priority Score with Respect to EPI

STEP 2	Soy-Bean	Rape Seed	Sunflower	Beef Tallow	EPI Score
Soy-Bean	0.50	0.47	0.62	0.30	0.47
Rape Seed	0.17	0.16	0.10	0.30	0.18
Sunflower	0.17	0.32	0.21	0.30	0.25
Beef Tallow	0.17	0.05	0.07	0.10	0.10

The net environmental indicator score for each alternative is calculated by the following formula.

$$Final\ Score = \sum(0.33 * A_i)$$

Where,

A_i = AHP score allotted to alternative with respect to environmental indicator i (i can be EPI, land usage or water usage)

0.33 = Score of importance given to environmental indicator i with respect to the other indicators (all indicators are given equal importance hence the score of 0.33). Table 24 A lists the environmental indicator score for each alternative calculated using the formula described above.

Table 23

Net Environmental Impact Score for Each Raw Material Alternative

	EPI	Land Usage	Water Usage	Environmental indicator score
Soy-Bean	**0.47**	**0.26**	**0.23**	**0.289**
Rape Seed	0.18	0.14	0.42	0.224
Sunflower	0.25	0.14	0.12	0.153
Beef Tallow	0.10	0.45	0.23	0.234

After performing the AHP calculations, soy-bean was identified to be the most favorable with respect to environmental implications as it has the highest environmental indicator score. AHP templates are also developed to quantify the other SD indicators and prioritize the raw materials with respect to economic (Zhang, Dube et al., 2003), safety and system specific indicators (NREL, 1994).

Table 24A

SD Indicator Quantification for Raw Materials

Alternatives	Economic		Safety		Fuel Performance	
	Total Costs($/kg)	Tot Manufacturing Cost of biodiesel $/L	RAM Index	Oxidation Stability (Rancimat Induction Period h)	Cetane Number	Carbon %
Soy Bean	0.52	0.3	LOW	5.9	51.34	0.94
Rape Seed	0.67	0.69	LOW	9.1	54.4	0.044
Sunflower	0.48	0.56	LOW	3.4	49	
Beef Tallow	0.3	0.85	MEDIUM	1.2	58	0.92

The net SD score is determined for each alternative by taking an aggregate of the product of the alternative's indicator score and the corresponding indicator's prioritization score for each SD indicator. The prioritization score for each SD indicator is calculated in the last column of Table 20. Table 24 B lists all the indicator scores for the raw material alternatives with respect to each SD indicator and the net SD score which is used to determine the most sustainable option. Soy-bean is considered the most sustainable raw material for bio-diesel production as it has an overall good performance in all the fields of SD.

Table 24 B

SD scores for Raw Material Alternatives

	Environmental	Economic	Safety	Fuel Performance	SD Score
Soy Bean	0.289	0.368	0.28	0.33	**0.32**
Rape Seed	0.224	0.145	0.37	0.23	0.22
Sunflower	0.153	0.240	0.24	0.31	0.23
Beef Tallow	0.234	0.247	0.12	0.13	0.19

7.2 Catalyst Selection

The transesterification process of bio-diesel can be catalyzed by homogenous catalysts which can be alkalis, acids or enzymes (Vicente., Martinez. et al., 2004). The first two types have received the greatest attention as they are more economically viable than enzyme catalyzed transesterification.

For this subsystem the SD indicators considered are environmental indicators (EPI), economic indicators (total manufacturing costs of biodiesel, break even price in $/tonne), safety indicators (RAM index) and certain system specific indicators such as reaction rime in minutes and percentage of yield. The quantification of these indicators is shown in Table 25.

Table 25

SD Indicators Quantification for Catalysts

Alternatives	Environmental	Economic			Safety		System Specific Indicators	
	EPI (for 100 units of release)	Total Costs ($ x10^{-6})	Tot Manufacturing Cost of biodiesel $ x 10^{-6}	Break Even Price ($/tonne)	RAM Index	Number Score	Reaction Time(min) for 90% conv	Yield %
Base (NaOH)	70	0.32	6.86	857	MEDIUM	2	90	95
Acidic(H2S04)	114.4	1.41	7.08	884	HIGH	3	4140	97
Enzyme	20	3.5	10.5	900	LOW	1	480	71

7.2.1 Prioritization of SD Indicators

For the catalyst subsystem, environmental and safety indicators are given high priority and the economic and system specific indicators are given medium priority. The prioritization scores obtained for each of SD indicators by AHP is displayed in Table 26.

Table 26

SD Indicators Prioritization Score

Indicator	Prioritization Score
Environmental	0.333
Economic	0.167
Safety	0.333
System Specific	0.167

7.2.2 Selection of Sustainable Alternative

The catalyst alternatives are compared with respect to each of the SD indicators. For environmental indicators the EPI values are determined for sodium hydroxide (NaOH) for alkaline catalyst (Vicente, Martinez. et al., 2004) and sulphuric acid (H_2SO_4) for acidic catalysts (Canakci and Van Gerpen, 1999). For economic indicators the percentage of difference in total manufacturing cost of bio-diesel and the bio-diesel break even price are used as comparison parameters (Zhang, Dube et al., 2003). With respect to safety implications, alkaline and enzymatic catalysts are comparatively safer than acid catalysts. Certain system-specific indicators such as reaction time (in min) and percentage of yield are used to compare the alternatives. Alkali catalyzed transesterification reactions are faster than acid or enzyme catalyzed reactions. Due to this reason, together with the fact that the alkaline catalysts are less hazardous and corrosive (inherently safer) than acid catalysts, industrial processes usually favor base catalysts (Zhang, Dube et al., 2003). However if the bio-mass used has a higher free fatty acid content and more water, acid-catalyzed transesterification is suitable. The results obtained for the most sustainable catalyst option by using the SD decision framework is displayed in Table 27.

Table 27

SD Scores for the Catalyst Alternatives

	Environmental	Economic	Safety	System Specific	SD Score
Base	0.478	0.549	0.54	0.48	**0.51**
Acidic	0.172	0.310	0.16	0.17	0.19
Enzyme	0.350	0.141	0.30	0.35	0.30

7.3 Reactant Alcohol Selection

The alcohols that can be used in the transesterification process are methanol, ethanol, propanol, butanol and amyl alcohol. Methanol and ethanol are used most frequently and hence are considered as the alternatives that are subjected to comparison for the identification of the more sustainable alcohol reactant.

The SD indicators used are the environmental indicators (EPI), economic indicators (total manufacturing cost of bio-diesel, break even price), safety indicators (RAM index) and fuel performance indicators (cetane number). The quantification of these indicators for the two alcohol reactant alternatives are shown in Table 28.

Table 28

SD Indicator Quantification for Alcohol Reactants

Alternatives	Environmental	Economic		Safety		Fuel Performance
	EPI (for 100 units of release)	Tot Manufacturing Cost of biodiesel $ x 10^{-6}	Break Even Price ($/tonne)	RAM Index	Number Score	Cetane Number
Ethanol	70	10	900	MEDIUM	2	48.12
Methanol	14	6.86	857	HIGH	3	51.34

7.3.1 Prioritization of SD Indicators

The prioritization of the SD indicators for the alcohol subsystem is shown in Table 29. In the transesterification reaction, the alcohol to triglyceride ratio is 6:1 for alkali catalyzed reaction and 30:1 for acid catalyzed. Due to the large amount of alcohol required, it affects the price of bio-diesel; hence economic indicator is given high priority. Environmental, safety and system specific indicators are given medium priority.

Table 29

Prioritization of SD Indicators for Alcohol Reactants

Indicator	Prioritization Score
Environmental	0.333
Economic	0.333
Safety	0.167
System Specific	0.167

7.3.2 Selection of Sustainable Alternative

Bio-diesel produced from ethanol and methanol have comparable chemical and physical fuel properties and engine performances (Peterson et al., 1995), but for economic reasons, only methanol is currently used for producing bio-diesel on an industrial scale due to the much lower price compared to ethanol. Methanol, however, is currently mainly produced from natural gas. Thus, methanol-based biodiesel is not a truly renewable product since the alcohol component is of fossil origin. Furthermore, methanol is highly toxic and hazardous, and its use requires special precautions. Use of ethanol for production of bio-diesel would result in a fully sustainable fuel, but only at the expense of much higher production costs. Table 30 illustrates the AHP scores obtained for the alcohol alternatives with respect to each of the SD indicators as well as the net SD score for each alternative. As can be seen in the table both the alternatives have the same SD score, but due to the above stated reasons, it is environmentally favorable and safer to use ethanol in the place of methanol though it is not a very economically favorable option.

Table 30

SD Score for Alcohol Alternatives

	Environmental	Economic	Safety	System Specific	SD Score
Ethanol	0.750	0.250	0.667	0.333	0.50
Methanol	0.250	0.750	0.333	0.667	0.50

7.4 Bio-diesel Production Process Selection

There are three most widely technologies to produce bio-diesel from plant oils or animal fats and they are pyrolysis, microemulsification and transesterification. Pyrolysis is the conversion of one substance into another by means of heat or by heat with the aid of a catalyst. it involves heating in the absence of air or oxygen and cleavage of chemical bonds to yield small molecules. The pyrolysis of vegetable oils, animal fats and natural fatty acids can result in the production of bio-diesel. Transesterification (also called alcoholysis) is the reaction of a fat or oil with an alcohol in the presence of a catalyst to form esters (bio-diesel) and glycerol. Micro-emulsion is the formation of thermodynamically stable dispersions of two usually immiscible liquids, brought about by one or more surfactants. But micro-emulsions of vegetable oils and alcohols cannot be recommended for long-term use in engines as they are prone to incomplete combustion, formation of carbon deposits and an increase in the viscosity of the lubricating oil. Due to these drawbacks micro-emulsions are not usually used in large-scale production of bio-diesel. In this study, only pyrolysis and transesterification processes are compared for the production of bio-diesel.

The SD indicators quantified for the production processes are the environmental (Impact degree), economic (total capital cost), safety (RAM index) and fuel performance (yield %) indicators. Table 31 shows the quantification of the SD indicators for the alternatives taken into consideration.

Table 31

SD Indicators for the Production Process Alternatives

Alternatives	Environmental	Economic	Safety	Fuel Performance
	Impact Degree	Total Capital Costs	RAM Index	Yield %
Thermal Cracking	HIGH	HIGH	HIGH	84
Transesterification	LOW	LOW	MEDIUM	98

7.4.1 Prioritization of SD Indicators

As the system under study is a process, economic and safety indicators are given high priority. As the environmental impact of the reactants involved in the process has already been included while selection the sustainable alternatives, environmental indicators are given only medium priority. System specific indicator (yield %) is given the least priority while comparing the different bio-diesel production techniques. Table 32 illustrates the AHP prioritization score for the SD indicators for the production process sub-system.

Table 32

Prioritization of SD Indicators for Production Process

Indicator	Prioritization Score
Environmental	0.189
Economic	0.351
Safety	0.351
System Specific	0.109

7.4.2 Selection of Sustainable Alternative

Transesterification has much better environmental and safety performance than thermal cracking as thermal cracking requires bio-diesel to be produced in an oxygen free environment and this requires more complex systems which increases the environmental impact as well as makes the process more hazardous (Ma and Manna, 1999). Moreover the bio-diesel obtained from transesterification has better emission performance than the bio-diesel obtained by thermal cracking. Transesterification is more economically favorable than thermal cracking due to lesser number of complex equipments. Due to all these favorable factors, transesterification is considered to be more sustainable than thermal cracking for producing bio-diesel. The AHP scores for each of the SD indicators as well as the final SD score for each alternative is shown in Table 33.

Table 33

SD Scores for the Production Process Alternatives

	Environmental	Economic	Safety	System Specific	SD Score
Thermal Cracking	0.33	0.33	0.33	0.18	0.32
Transesterification	0.67	0.67	0.67	0.83	**0.68**

7.5 Bio-diesel Purification Process Selection

Bio-diesel purification method is the final subsystem considered in this case study. The alternatives considered are water washing and hexane extraction. Due to the evident impact of this subsystem on the total cost of bio-diesel, the economic implications are given the highest priority followed by safety issues. The reasoning for the priority scores allotted for environmental and system specific indicators is similar to that offered for the bio-diesel production process subsystem. Table 34 shows the SD indicator prioritization scores. Water washing has a much better environmental performance than hexane extraction due to the avoidance of use of hexane thereby making the process inherently safer (Zhang, Dube et al., 2003). Though hexane extraction can yield more pure bio-diesel, it is not required unless acid catalyzed, used vegetable oil or similar more contaminated feed stock is used as a raw material. Water washing is also economically favorable than hexane extraction due to simpler equipment and more readily available materials (water is cheaper and readily available than hexane). Due to these favorable features, water washing is usually preferred to hexane extraction and this was the result obtained from the decision framework developed. Table 35 shows the SD scores for the bio-diesel purification process alternatives.

Table 34

Prioritization of SD Indicators for Bio-Diesel Purification

Indicator	Prioritization Score
Environmental	0.189
Economic	0.351
Safety	0.351
System Specific	0.109

Table 35

SD Scores for the Bio-Diesel Purification Process Alternatives

	Environmental	Economic	Safety	System Specific	SD Score
Water washing	0.75	0.75	0.67	0.24	**0.67**
Hexane Extraction	0.25	0.25	0.33	0.76	0.33

The final bio-diesel system with the identified sustainable alternatives for each subsystem is illustrated in Table 36. The list of alternatives identified to be the most sustainable by the proposed methodology agrees closely with the generic system accepted to be the most optimal and environmentally favorable by most researchers and commercial bio-diesel plant designers. This proves the effectiveness of the proposed methodology.

Table 36

Sustainable Bio-Diesel Process

Subsystem	Sustainable Alternative
Bio mass	Soy-Bean
Catalyst	Basic
Alcohol	Ethanol
Production process	Transesterification
Bio-diesel Purification	Water Washing

8 FUTURE WORK AND CONCLUSION

8.1 Conclusion

The method elucidated here is an analytical approach to sustainable engineering decision making. The decisions made regarding the bio-diesel production alternatives aim at identifying the most sustainable process taking into account environmental, economical and safety implications. The SD decision framework results for the most sustainable bio-diesel process in this paper are similar to the alternatives that are considered to be economically and environmentally favorable by both researchers and commercial manufactures (Zhang et. al., 2002; Haas et. al., 2005; NREL). This demonstrates that the proposed methodology takes into consideration the factors that are considered important in making decisions regarding suitable bio-diesel production alternatives. Due to this feature of the decision framework, a commercial manufacturer of bio-diesel will be able to use the proposed methodology for making a more complete sustainable development. The developed framework is user friendly and can be customized by altering the scoring scales used in prioritizing the SD indicators and for the comparison of alternatives. The framework can be altered to accommodate more bio-diesel subsystems to be included in the sustainable development.

The framework can also be customized to be applied to systems other than bio-diesel, as the scoring scales for the SD indicators and alternatives comparison are not very system specific. Hence the framework developed is simple, flexible and acceptably accurate in identifying sustainable options from a given set of alternatives.

8.2 Future Work

To further improve the decision making, social implications can also be included in the future versions of the SD decision making framework. Issues such as tax incentives, employment generation, and revenue generation for cultivators will be included in the social sustainability metrics. Though these metrics cannot be directly used as comparison parameters in an AHP template, they can be converted into economic terms such as costs or returns and then used as comparison parameters.

Inclusion of social indictors in the proposed framework will complete the SD of the process under consideration as the decisions made regarding the alternatives within each subsystem, will cover economic, environmental, safety and social implications. Currently the comparison scales defined for the prioritization of the SD indicators and the subsystem alternatives are defined based on historic data, to further improve the accuracy of these scales a sensitivity analysis can be performed to analyze the effect of the AHP comparison scales on the SD decisions made for the bio-diesel system. Similarly the extent of the effect of the priority scores of the SD indicators on the decision regarding the most sustainable alternative for each subsystem can be identified by performing a sensitivity analysis on the SD prioritization score. These sensitivity analyses will provide a more detailed understanding of the proposed SD decision making technique and an opportunity to improve the accuracy of the technique with respect to the selection of sustainable alternatives.

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