Economic Risk Analysis and Environmental Life Cycle Assessment of Bio-energy Systems

by

©Zaman Sajid

A thesis submitted to the
School of Graduate Studies
in partial fulfillment of the requirements for the degree
of

Doctor of Philosophy (Ph.D.)

Faculty of Engineering and Applied Science

Memorial University of Newfoundland

October 2017

St. John's Newfoundland

Key words

Process Economics, Economic risk analysis, Cost uncertainty, Probabilistic Cost, Probabilistic Revenue, Environmental Friendly Fuel, Biodiesel System, Risk Analysis, Safety Analysis, Interpretive Structural Modelling, Dependence Analysis, Process Economics, Risk Model, Value at Risk, Biodiesel Production, Interpretive Structural Modelling, Environmental Load, Energy Sustainability, Biodiesel Process Simulation, Life Cycle Assessment, Life Cycle Thinking, Biodiesel Policy-making

Abstract

Being depletable, scarce, hostile to the environment and non-renewable in nature, petroleum-based fossil fuels are diminishing much faster than a decade ago. These scarcity concerns, negative environmental consequences and the gradual depletion of petroleum fuels have led to explore alternate, inexhaustible and renewable energy resources. One promising energy resource is biofuel, which is produced from renewable biomass feedstock. The reasons for sustainability and viability of biofuels are that they are economically feasible to produce and have positive environmental impacts. Since biofuels research is quite diversified, the sustainability and viability of biofuels face many challenges. This thesis investigates existing and future technological and knowledge challenges and proposes new methods to improve bio-energy sustainability both economically and environmentally. The economic viability of biofuels is associated with biofuel cost estimation, the revenue earned, and the profit gained. This research evaluates the cost risk escalation and identifies the key cost factors associated with the economic viability of biofuels. To achieve this objective, this research presents an innovative methodology to perform probabilistic economic risk analysis of biofuel, and particularly biodiesel. Being stochastic in nature, the proposed methodology addresses the shortcomings of traditional biodiesel process economics and provides flexibility to deal with uncertainty in biodiesel process economics. The environmental aspects covered in this research are environmental impacts caused by all inputs to the biodiesel production process, including biomass feedstock, fresh or recycled materials and energy streams and outputs such as biodiesel, by-products and waste materials discharged into the soil and air.

To address the influences of potential risks on biodiesel production and its environmental impacts, this thesis presents a new approach to perform probabilistic economic modelling, qualitative and quantitative risk assessment of biodiesel key performance indicators (KPIs) and life cycle assessment (LCA) of biodiesel fuel. Interpretive structural modelling (ISM) is used to model causation behaviour of the biodiesel process, operations and design risk factors. The basic premise of ISM is that qualitative interdependent relationships among various risk factors are achieved through experts' opinions and a scientific approach. This thesis develops an objective risk analysis approach to integrate ISM and uses a Bayesian network (BN) to define the relationship and the strength of relationship among various cost related risk factors and studies their impact on biodiesel process economics.

Addressing global environmental issues and considering the vital need of edible oil for food, this thesis also presents the LCA of biodiesel being produced from inedible oils and waste cooking oil (WCO) and performs the investigation using a systematic approach of life cycle thinking. The negative environmental consequences of biodiesel fuels on climate change (global warming), ecosystem quality and human health are explored in detail. The study also identifies the total environmental impacts of using these biomass feedstocks. A comparative LCA study of technological processes identifies which biodiesel production process has the most and the fewest ecological impacts and energy requirements.

Finally, this research develops advanced methods for biodiesel process economics such as process value at risk (VaR), to be used in assessing the performance of biodiesel systems. The stochastic modelling process and interdependence of a BN format help to investigate the most significant risk factors in the biodiesel process and operations. The results facilitate the decision-making process for new product development (NPD) and process development, especially at a large industrial scale.

Applications of the proposed economic risk assessment framework along with an LCA study help to develop effective biodiesel policy-making by describing scientific uncertainties related to process economics and the environmental impact of biodiesel production technologies. In another arena of application, this thesis helps to develop a strategic decision-making process for supply chain management of biomass feedstock as well as biodiesel. It also enhances the biodiesel process-based risk informed decision-making process by incorporating techno-economic and life cycle accounting decisions.

Statement of original authorship

I state that the work contained in this thesis is original and has not been previously submitted to fulfil the partial/full requirements of a degree or diploma at any other higher education institution other than the Department of Process Engineering, Faculty of Engineering and Applied Science, Memorial University of Newfoundland, St. John's, Newfoundland, Canada.

To the best of my knowledge, this thesis does not breach copyright law, or contain any material previously published or written by another person except where due reference is made in text. I declare that the material in this thesis is my own work and due acknowledgment has been made where contributions are made by supervisors.

Signature: Zaman Sajid

Date: August 22, 2017

Acknowledgements

I would like to express my thanks and gratitude towards my honourable supervisors Dr. Faisal Khan and Dr. Yan Zhang for their guidance, leadership, support, excellent mentorship during this journey of Ph.D. studies. I am thankful to both of them for providing me an opportunity to explore sustainable energy concepts through Ph.D. studies. I would like to express special thanks to Dr. Faisal Khan for all his patience while I prepare for updates. His wise leadership, patience and prompt feedback helped me to learn too many new things and were a continuous source of encouragement to complete this journey through enthusiasm and determination. I am thankful to him for his constructive criticism and helpful discussions in improving this thesis.

Tremendous gratitude is due to the guidance, encouragement and mentorship of Dr. Yan Zhang. She has always been present when I need her support and help. She has not only been a source of continues support in my research but also improved my paper writing skills. Her insightful comments and advices helped me to overcome many challenges and finish this thesis.

I am also truly indebted to Dr. Syed Imtiaz, a member of my supervisory committee, for his advices on my Ph.D. exams preparations and research planning and development.

I am thankful to Memorial University of Newfoundland for financially supporting my studies. My sincere gratitude is also due to Moya Croker and Collen Mahoney in engineering graduate office and Memorial University library staffs especially engineering librarian Dianne Taylor-Harding and Aspi Balsara for their support and care. Gratitude is also extended to Beverley Brown for her academic editing and proofreading of my thesis. I am also thankful to Munaza Younas for her support and encouragement while I focus on my studies. I am also thankful to my uncle Rana Naveed in taking care of my family while I am away from home.

This thesis is dedicated to my late father Mr. Sajid Mahmmod, mother Mrs. Rukhsana Sajid, my siblings Waseem Sajid and Shameel Sajid.

Table of Contents

List of Tables

List of Figures

List of Acronyms and Symbols

A(si)	Antecedent set
AFC	Annual fixed cost
AOC	Annual operating cost
B	Benefit
BN	Bayesian network
C	Cost
CBA	Cost benefit ratio analysis
CEPCI	Chemical Engineering Plant Cost Index
CO_2	Carbon dioxide
CPR	Closed pond photo-bioreactor
CPT	Conditional probability table
DAG	Directed acyclic graph
EPC	Energy Performance Contracting
FAME	Fatty acid methyl ester
FC	Fixed cost
FCC	Fixed Capital Cost
FCI	Fixed capital investment
FFA	Free fatty acid
gal	Gallon
GHG	Greenhouse gas emissions
h	Hour
HC	Hydrocarbon

HYSYS	HYprotech SYStems
$I_{fraction}$	Fractional contribution
IPCC	International Panel on Climate Change
ISM	Interpretive structural modelling
ISO	International Organization for Standardization
KM	knowledge management
KPIs	key performance indicators
l	Litre
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
M	Million
MGPY	Million gallons per year
NNP	Net annual profit after taxes
NPD	New product development
NPV	Net Present Value
P	Probability
PAHs	Polycyclic aromatic hydrocarbons
PCE	Purchase cost of major equipment
PFC	Plant Fixed Capital
PFD	Process flow diagram
PWC	Plant Working Capital
R	Revenue
R(si)	Reachability set

RM	Reachability matrix
ROI	Return-on-investment
SCOR	Supply-chain operations reference
SSIM	Structural self-interaction matrix
t	Ton
TC	Total cost
TCI	Total capital investment
TCI	Total Capital Investment
TPC	Total production cost
TPM	Total productive maintenance
TZS	Tanzanian shillings
UNIQUAC	Universal quasi-chemical
VaR	Value at risk
VC	Variable cost
VE	Variable elimination
WCO	Waste cooking oil
WVO	Waste vegetable oil
$\cap$	Intersection

Chapter 1

1 Introduction

1.1 An overview of biodiesel production

With the steady use and gradual depletion of fossil fuel resources, and their adverse environmental impacts, research is being focused on developing alternative fuels which are environmentally friendly and renewable. One of these sustainable alternatives is biodiesel – an alternate fuel to petroleum-based diesel fuel. To make it commercially viable, there are two kinds of challenges in biodiesel commercialisation: first, the technological maturity of the biodiesel production process, and second, its process economics. Previously, in-depth research has been conducted on the technological maturity of the biodiesel production process (Ma and Hanna 1999, Antolín, Tinaut et al. 2002, Boehman 2005) which demonstrates the production of biodiesel through a chemical reaction of vegetable oil and animal fats with an alcohol, in the presence of a catalyst. The catalyst is usually a strong base (potassium or sodium hydroxide) and the reaction produces two products: methyl ester and glycerol. Methyl ester is called biodiesel (Van Gerpen 2005). The renewability of biodiesel comes from two facts: first, from the renewable feedstock being used to produce biodiesel. Generally, the feedstock could be either vegetable oils, animal fats or waste cooking oils. These feedstocks are mostly developed by consuming atmospheric carbon dioxide and thus the biodiesel produced has less contribution to global warming than fossil fuel resources (Borugadda and Goud 2012). Second, there are much fewer net carbon dioxide emissions from the combustion of biodiesel compared to the combustion of petroleum-based diesel. A study showed a net decrease of 78% of carbon dioxide content using biodiesel as a combustion fuel, compared to using petroleum based diesel (Sheehan, Camobreco et al. 1998). Vegetable oils and animal fats are high in viscosity and therefore cannot be used directly as a fuel in a diesel combustion engine (Goering, Schwab et al. 1982). Special processes are adopted through which the vegetable oils and/or animal fats are converted into useable biofuels for a diesel combustion engine. These processes are:

I. Direct use and blending of vegetable oils with diesel fuel (Koh and Ghazi 2011)
II. Micro-emulsion of oils (Balat and Balat 2010)
III. Pyrolysis of oils (Lappi and Alén 2011)
IV. Trans-esterification (Marchetti, Miguel et al. 2007)

On an industrial scale, trans-esterification is the most common technology to produce biodiesel (Abbaszaadeh, Ghobadian et al. 2012). The trans-esterification reaction helps to reduce the viscosity of oils and fats by converting them into methyl esters (Abbaszaadeh, Ghobadian et al. 2012). To produce biodiesel, the trans-esterification reaction is accomplished either in the presence or absence of catalysts (Demirbas 2005, Demirbas 2009). The physical phase of the catalyst could be a homogeneous one, such as potassium hydroxide, sodium hydroxide, or sulphuric acid (Vicente, Martınez et al. 2004), or it could be heterogeneous (Helwani, Othman et al. 2009), including lipases (Fan, Niehus et al. 2012), magnesium oxide (Demirbas 2008) or calcium oxide (Liu, He et al. 2008). Considering the raw material, also called biomass for biodiesel production, there are varieties of feedstock being used and many are in research phase. In this regard, a general classification is made among edible oils, non-edible oils and biomass wastes (Meher, Sagar et al. 2006). The production, use and properties of different biomasses have been reported in the literature (Atabani, Silitonga et al. 2012).

1.2 Biodiesel process economics

As is evident from the discussion in the previous section, the process of biodiesel production has been well-addressed in the literature. To summarize this, there are various production technologies, different catalysts, and a diversified range of biomass feedstock that can be used to produce biodiesel. However, on an industrial scale, only those processes or combination of processes are chosen which have potential to produce biodiesel in an economical way. Therefore, most biodiesel economic research is diversified in nature and estimates various economic parameters of biodiesel production using different biodiesel production technologies, biomass feedstock, and chemical processes. (Nagarajan, Chou et al. 2013, Ang, Tan et al. 2014). Generally, the literature on biodiesel process economics represents the cost of biodiesel production, the design and technical route adopted to produce biodiesel, the capital investment needed, how the plant is economically managed and the expected annual profit for a given plant capacity, as presented in Table 1.1.

Table 1.1 Biodiesel economics analysis

Feedstock type	Plant capacity and the process technology	Production cost	Prices	Expected Profit	Reference
Soy oil	40 MGPY Trans-esterification	Fixed capital investment (FCI) = $17,779,000 Annual fixed cost (AFC) = $2,072,000/year Annual operating cost (AOC) minus feedstock cost = $16,970,000/year	Feedstock soy, $0.49/lb Biodiesel price = $2.88/gal (year 2008)	$2.67M/year	(Elms and El-Halwagi 2010)
Jatropha oil	1-ton biodiesel Alkali catalysed trans-esterification	Total capital investment (TCI) = $ 13,908 Total production cost (TPC) – variable cost = $2,059 Total production cost (fixed cost and general expenses) = $1,455	Cost of jatropha oil = $0.191/litre (year 2008) Estimated biodiesel cost = $1.02/litre	$803/day	(Ofori-Boateng and Lee 2011)

Waste cooking oil (WCO)	40 MGPY Trans-esterification process	Fixed capital investment =$22,479,000 Annual fixed cost (AFC) = $2,972,000/year Annual operating cost (AOC) minus feedstock cost = $19,089,000/year	WCO (50% FFA) = $0.20/lb Biodiesel = $2.88/gal (year 2008)	$3.37M/year	(Elms and El-Halwagi 2010)
Microalgae	Closed pond photo-bioreactor (CPR) Biomass productivity = 39.2 ton/day	Total capital investment = $44.68M	Oil = $18.35/gal Biodiesel = $21.11/gal	Revenue = $21.96 M/year	(Ramos Tercero, Domenicali et al. 2014)
Soybean oil	8000 tons/year	Feedstock cost = $779/ton	Biodiesel cost = $0.780/l	Net annual profit after taxes (NNP) = $($24x10^3$)	(You, Shie et al. 2008)

1.3 What is missing?

Economic analyses of biodiesel production provide a detailed overview of the economics of a biodiesel production system. This estimated cost-revenue data can help investors to estimate profitability from biodiesel plant construction and operations. Despite these detailed economic studies, most biodiesel projects have either failed in their execution or the projects had to bear tremendous losses. Some of these studies are presented below.

In 2008, Enerkem started construction of a biofuel plant named Enerkem Alberta Biofuels in Edmonton, Canada. The project aimed to convert the municipal solid waste of the city of Edmonton into biofuel. The plant, with a capacity of 10 million gallons per year and cost of $80 million, was supposed to be built by 2012; however, due to various factors, the project cost jumped to more than $100 million with a plant production delay period of two years. The factors which affected the production and economics of the plant were design changes, the application of an innovative technology to produce biofuel on a large-scale, re-engineering of previously approved engineering designs, and nonconformity to specifications from contractors and suppliers (Bascaron 2016).

In 2009, Sun Biofuels UK launched a biodiesel project in the District of Kisarawe, Tanzania. The plant was slated to produce biodiesel from jatropha and the investors acquired more than 8,211 hectares of land. The company planned to invest $20 million (25.3 billion TZS). But after two years many factors, which investors did not include in their economic studies, brought the project to a complete shutdown. These were bankruptcy, internal organizational changes, change of top management, nonretention of key personnel and non-compliance with land acquisition regulations (Bergius 2012).

In 2008, Clovis Biodiesel, an Australian company, had to delay the construction of a biodiesel plant which aimed to produce biodiesel from animal feedstock such as beef tallow. The plant was located in New Mexico USA, and had a capacity of 75 million gallons of biodiesel production a year, with an estimated cost of $18 million. The company had to delay plant construction and subsequently biodiesel production was delayed due to the price fluctuations of animal feedstock and the land transfer non-compliance with the local government (Monte 2008, Watch 2008).

To construct and operate an advanced bio-refinery, there is a need to spend billions of dollars as capital investment and to meet the operational expenditures. As of 2013, Canadian biofuel industries have spent 2.3 billion dollars in constructing 23 biodiesel plants which produce about 956 million litres of biodiesel annually (Webb 2013). In order to estimate such an investment, process engineers rely on process economics techniques available in the literature where fundamental loopholes are present in cost estimation techniques. Although biodiesel economic studies were performed in all aforementioned projects, these projects had either exceeded cost or had a delay in biodiesel production start-up; which affected the process economics and subsequently the return period. An analysis of causes of these projects' failures and the literature (Sinnott, Richardson et al. 2013) reveals that the currently available process economics studies in the literature are lacking in the following two dimensions:

I. These studies do not provide the level of accuracy for the cost and revenue data used, and hence introduce an uncertainty in cost and revenue data.

II. These studies do not show how biodiesel performance risk factors may affect monetary variables such as costs, revenues and associated profits.

Considering these two dimensions of economic analysis, one can have a holistic picture of the biodiesel system performance and the expected profit. Since many technological innovations of biodiesel production and processes are in their early stages of innovation therefore many uncertainties have been introduced in biodiesel economic analysis. Biodiesel performance risk management depends on the risks developed by such uncertainties in a biodiesel economic analysis.

1.4 Research background and problem statement

To produce biodiesel on an industrial scale, the production technology should be commercially viable and the process and operation should have the ability to generate profit. In the current scenario of biodiesel market fluctuations, changes in the prices of petroleum-based diesel and the vague future aspects of biodiesel use, this profit is not risk free. The quantification of loss for a given investment is the key to financial risk management. Nonetheless, accurate quantification of such risks is a big challenge due the complexity of the biomass and issues related to producing, harvesting, and transporting and processing the biomass. The performance of a biodiesel facility is affected by various risk factors, which directly or indirectly influence biodiesel investment decisions. Therefore, understanding the nature of such biodiesel performance risks factors, their relative strength and their impact on biodiesel economic decisions is important to develop sustainability in biodiesel process economics. So far, the nature of these risk factors has not been studied and explored. Moreover, the qualitative as well as the quantitative interdependency of such risks and their impacts on biodiesel process economics have not been studied. The identification of these risk factors and their interdependent influence on biodiesel process economics is vital to establish an effective biodiesel performance based risk management system. Thus, there is a need to develop a methodology to perform biodiesel performance analysis by incorporating financial risk management tools. Uncertainty in process economic data introduces a risk of cost escalation in execution of a biodiesel project, which increases the risk of making a biodiesel project unprofitable. Technically speaking, such attributes introduce two major research gaps in biodiesel process economic analysis: the presence of uncertainty in cost and revenue data and the variability associated with biodiesel performance risk factors.

I. The presence of uncertainty in cost and revenue data

The vagueness in biodiesel process economics could be due to the presence of uncertainty in the biodiesel cost and revenue data. To perform an economic analysis of a biodiesel production plant on an industrial scale, the values for cost estimation and revenue estimation would be in the hundreds of millions of dollars and an uncertainty of, even, 1% could lead to either cost underestimation or budget nonconformity, which could substantially affect the biodiesel profit. Hence, this necessitates a probabilistic economic risk analysis for a biodiesel system.

II. Variability associated with biodiesel performance risk factor

The profit reported for a biodiesel production plant could also change with the variability associated with biodiesel performance risk factors. The performance of a biodiesel production plant is highly dependent on various risk factors, for example, process design accuracy, supply chain risks, likelihood of process change and many more. The inclusion of such risk factors in the economic study of biodiesel production can be accurately reflected in an economic analysis. Unfortunately, as of today no research has been performed to develop such a methodology.

From the product sustainability point of view, there are three pillars of sustainability, which include economic, environmental and social aspects of a product. Considering the environmental pillar of sustainability, life-cycle assessment (Malça, Coelho et al. 2014) is a useful tool to determine the environmental sustainability of biodiesel production systems. LCA is a well-established and comprehensive methodology to find the adverse environmental and human health impacts of a product which occur throughout its life cycle (Allen and Shonnard 2001). The life cycle of biodiesel includes the extraction of raw materials, transportation of raw material to the production site, product manufacturing, the transportation of the product to market, its use and disposal at its end of life. The whole objective of the analysis is to determine the adverse environmental impacts of biodiesel. As various processes and methodologies can be utilized for biodiesel production, this introduces a need to evaluate which production method and raw material would potentially have a considerable environmental impact. The results obtained would subsequently help to make an informed decision about the most environmentally friendly production method and raw material to produce biodiesel. Other than identification of adverse environmental impacts of biodiesel production, the LCA tool can also help in decision making pertaining to biodiesel and biomass supply chain management.

1.5 Research scope and objectives

The scope of this research covers both the economic and environmental pillars of sustainability for a biodiesel production system. But, the social impacts of biodiesel production system are not covered in this thesis. The scope of the economic pillar includes the variability associated with the cost and revenue data. The probabilistic risk analysis includes the probabilistic cost risk analysis, probabilistic revenue risk analysis and probabilistic risk analysis of the major equipment being used to produce biodiesel. Production equipment with a lower cost is not within the scope of this thesis. The economic analysis is based on a biodiesel plant using non-edible oil, obtained from Jatropha curcas and the environmental LCA is based on a biodiesel plant using waste cooking oil (WCO) as biomass feedstock. In comparative LCA analyses, the plant has a production capacity of 45,000 tonnes per year and biodiesel is being produced by trans-esterification reaction. The catalyst for the chemical reaction is sodium hydroxide, while methanol is used as an alcohol in the trans-esterification reaction. The models developed in this work have their applications in biodiesel process economics decisions, where a techno-economic analysis is being performed to assess the commercial viability of biodiesel production, especially when an innovative process and new biomass feedstock are being used. The proposed models in this thesis perform analyses to answer the following questions:

- How much could cost escalate from the estimated one in producing biodiesel?
- How much revenue could be affected based on market demand for biodiesel?
- Which equipment has significant cost uncertainty in producing biodiesel?
- What are the factors affecting the performance of a biodiesel system?
- How are biodiesel performance risk factors related to each other?
- How much of an impact could biodiesel cost risk factors make on overall profit?
- If the cost of a biodiesel plant escalates, what will be the consequences?
- How clean is the energy fuel of biodiesel if produced from wastes?

With these questions in mind, this thesis aims to:

- Develop an economic risk analysis methodology which could deal with uncertainties in biodiesel estimated cost and revenue data by incorporating probabilistic economic risk analysis and commercial viability assessment of biodiesel production system with the risk of cost escalation.
- Establish a network approach for both qualitative and quantitative analyses of biodiesel performance risk factors, their interdependency and impacts on biodiesel process economics.
- Perform comparative environmental life cycle assessment of two biodiesel production systems.

1.6 Organization of the Thesis

This thesis is divided into four phases and consists of seven chapters. The organization of thesis is presented in Figure 1.1 which shows the link of each chapter with research contributions in a cohesive way.

Phase one primarily consists of Chapter 1, which provides an introduction to the thesis. This starts from a review of the current available techniques in biodiesel process economics and identifies what is missing so far. Then it defines the problem statement by identifying the research gap between the existing process economics methods and the causes behind the failure of various industrial projects. Next, it provides the contributions and research objectives and briefly summarises the research innovations in the proposed methodology in this thesis.

Phase two mainly consists of Chapter 2, which is a literature review and outlines the history of available biodiesel process economics and environmental impact assessment techniques. It reviews the existing literature and identifies the research gaps present in current biodiesel process economics and environmental studies. This phase also discusses the basic principles that will be used to address some of the major issues identified in the problem statement of this thesis.

Phase three of the thesis consists of Chapters 3, 4, 5 and 6, and presents thorough and comprehensive investigation techniques associated with biodiesel commercialization and greenhouse gas effects. Chapter 3 proposes an innovative economic risk-based model for a biodiesel facility using stochastic modelling. This chapter develops and highlights the methodological framework for probabilistic risk analysis and shows its applications in a biodiesel facility. The cost-benefit analysis identifies the project's benefits using various scenarios. Chapter 4 presents a methodology to study the interdependence of various risk factors affecting the performance of a biodiesel system. An integrated technique, developed by the integration of a Bayesian network and interpretative structural modelling, shows the level of hierarchy for various risk factors. Chapter 5 presents an integrated economic model which is developed using Monte Carlo Simulation performed on cost-revenue data. The economic model incorporates the impacts of cost risk factors, identified by a literature search and initially correlated by a group of experts' opinions. Chapter 6 presents the policy-making application for commercialisation of biodiesel through its life cycle assessment study. This chapter highlights the challenges of biodiesel production using waste materials and discusses their environmental impacts. Originally, Chapters 3, 4, 5 and 6 were first written as separate journal articles and Chapters 3, 4 and 6 have already been published, while Chapter 5 is currently under review for a possible publication.

Finally, phase four of the thesis in Chapter 7 includes the major conclusions drawn from this research along with recommendations for future research work. This phase also highlights the innovative contributions made by this thesis in the field of sustainable energy. Phases one, two and three also contain the references consulted in the chapters inside.

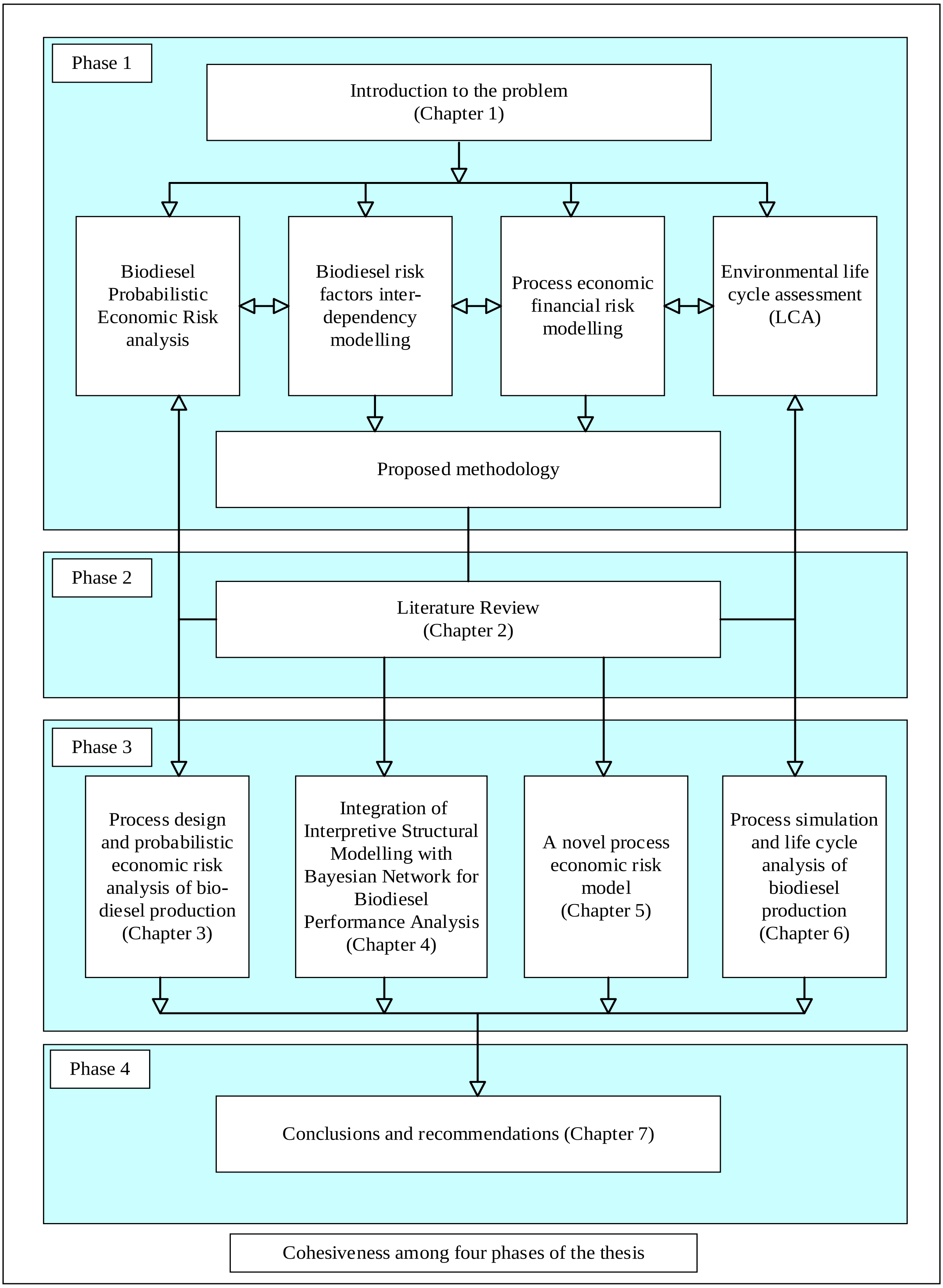


Figure 1.1 Schematic diagram of research methodology in thesis

1.7 References

Abbaszaadeh, A., B. Ghobadian, M. R. Omidkhah and G. Najafi (2012). "Current biodiesel production technologies: a comparative review." Energy Conversion and Management 63: 138-148.

Allen, D. T. and D. R. Shonnard (2001). Green engineering: environmentally conscious design of chemical processes, Pearson Education.

Ang, G. T., K. T. Tan and K. T. Lee (2014). "Recent development and economic analysis of glycerol-free processes via supercritical fluid transesterification for biodiesel production." Renewable and Sustainable Energy Reviews 31: 61-70.

Antolín, G., F. V. Tinaut, Y. Briceño, V. Castaño, C. Pérez and A. I. Ramírez (2002). "Optimisation of biodiesel production by sunflower oil transesterification." Bioresource Technology 83(2): 111-114.

Atabani, A. E., A. S. Silitonga, I. A. Badruddin, T. M. I. Mahlia, H. H. Masjuki and S. Mekhilef (2012). "A comprehensive review on biodiesel as an alternative energy resource and its characteristics." Renewable and Sustainable Energy Reviews 16(4): 2070-2093.

Balat, M. and H. Balat (2010). "Progress in biodiesel processing." Applied Energy 87(6): 1815-1835.

Bascaron, S. (2016). "Enerkem biofuel plant, backed by City of Edmonton, mired in legal controversy." Retrieved Feb 5, 2017, from http://www.cbc.ca/news/canada/edmonton/enerkem-biofuel-plant-backed-by-city-of-edmonton-mired-in-legal-controversy-1.3509177.

Bergius, M. (2012). Understanding land investment deals in Africa: Tanzanian villagers pay for Sun Biofuels investment disaster. Oakland, The Oakland Institute: 1-9.

Boehman, A. L. (2005). "Biodiesel production and processing." Fuel Processing Technology 86(10): 1057-1058.

Borugadda, V. B. and V. V. Goud (2012). "Biodiesel production from renewable feedstocks: Status and opportunities." Renewable and Sustainable Energy Reviews 16(7): 4763-4784.

Demirbas, A. (2005). "Biodiesel production from vegetable oils via catalytic and non-catalytic supercritical methanol transesterification methods." Progress in energy and combustion science 31(5): 466-487.

Demirbas, A. (2008). "Biodiesel from Vegetable Oils with MgO Catalytic Transesterification in Supercritical Methanol." Energy Sources, Part A: Recovery, Utilization, and Environmental Effects 30(17): 1645-1651.

Demirbas, A. (2009). "Biodiesel from waste cooking oil via base-catalytic and supercritical methanol transesterification." Energy Conversion and Management 50(4): 923-927.

Elms, R. D. and M. M. El-Halwagi (2010). "The effect of greenhouse gas policy on the design and scheduling of biodiesel plants with multiple feedstocks." Clean Technologies and Environmental Policy 12(5): 547-560.

Fan, X., X. Niehus and G. Sandoval (2012). Lipases as Biocatalyst for Biodiesel Production. Lipases and Phospholipases: Methods and Protocols. G. Sandoval. Totowa, NJ, Humana Press: 471-483.

Goering, C. E., A. W. Schwab, M. J. Daugherty, E. H. Pryde and A. J. Heakin (1982). "Fuel Properties of Eleven Vegetable Oils." 25(6).

Helwani, Z., M. Othman, N. Aziz, J. Kim and W. Fernando (2009). "Solid heterogeneous catalysts for transesterification of triglycerides with methanol: a review." Applied Catalysis A: General 363(1): 1-10.

Koh, M. Y. and T. I. M. Ghazi (2011). "A review of biodiesel production from Jatropha curcas L. oil." Renewable and Sustainable Energy Reviews 15(5): 2240-2251.

Lappi, H. and R. Alén (2011). "Pyrolysis of vegetable oil soaps—palm, olive, rapeseed and castor oils." Journal of Analytical and Applied Pyrolysis 91(1): 154-158.

Liu, X., H. He, Y. Wang, S. Zhu and X. Piao (2008). "Transesterification of soybean oil to biodiesel using CaO as a solid base catalyst." Fuel 87(2): 216-221.

Ma, F. and M. A. Hanna (1999). "Biodiesel production: a review." Bioresource Technology 70(1): 1-15.

Malça, J., A. Coelho and F. Freire (2014). "Environmental life-cycle assessment of rapeseed-based biodiesel: Alternative cultivation systems and locations." Applied Energy 114: 837-844.

Marchetti, J., V. Miguel and A. Errazu (2007). "Possible methods for biodiesel production." Renewable and sustainable energy reviews 11(6): 1300-1311.

Meher, L., D. V. Sagar and S. Naik (2006). "Technical aspects of biodiesel production by transesterification—a review." Renewable and Sustainable Energy Reviews 10(3): 248-268.

Monte, G. (2008). "Feedstock Costs, Capital Raising Woes Delay Construction of Clovis, New Mexico Biodiesel Plant." Clovis News Journal Retrieved March 12, 2017, from http://www.soyatech.com/news_story.php?id=7236.

Nagarajan, S., S. K. Chou, S. Cao, C. Wu and Z. Zhou (2013). "An updated comprehensive techno-economic analysis of algae biodiesel." Bioresource Technology 145: 150-156.

Ofori-Boateng, C. and K. T. Lee (2011). Feasibility of Jatropha oil for biodiesel: Economic Analysis. World Renewable Energy Congress-Sweden; 8-13 May; 2011; Linköping; Sweden, Linköping University Electronic Press.

Ramos Tercero, E. A., G. Domenicali and A. Bertucco (2014). "Autotrophic production of biodiesel from microalgae: An updated process and economic analysis." Energy 76: 807-815.

Sheehan, J., V. Camobreco, J. Duffield, M. Graboski and H. Shapouri (1998). Life cycle inventory of biodiesel and petroleum diesel for use in an urban bus. Final report, National Renewable Energy Lab., Golden, CO (US).

Sinnott, R. K., J. F. Richardson and J. M. Coulson (2013). Chemical Engineering: An Introduction to Chemical Engineering Design, Elsevier Science.

Van Gerpen, J. (2005). "Biodiesel processing and production." Fuel processing technology 86(10): 1097-1107.

Vicente, G., M. Martınez and J. Aracil (2004). "Integrated biodiesel production: a comparison of different homogeneous catalysts systems." Bioresource technology 92(3): 297-305.

Watch, M. (2008). "Construction Delayed On Biodiesel Plant Planned For Clovis, NM." Retrieved March 13, 2017, from http://www.marketwatch.com/story/construction-delayed-on-biodiesel-plant-planned-for-clovis-nm-2008-03-11.

Webb, A. (2013). "What does it takes to build an advanced biofuels plant?" Biofueled - a blog about advanced biofuels, retrieved March 13, 2017, from http://www.biofuelnet.ca/2013/08/07/what-does-it-take-to-build-an-advanced-biofuels-plant/.

You, Y.-D., J.-L. Shie, C.-Y. Chang, S.-H. Huang, C.-Y. Pai, Y.-H. Yu and C. H. Chang (2008). "Economic Cost Analysis of Biodiesel Production: Case in Soybean Oil." Energy & Fuels 22(1): 182-189.

Chapter 2

2 Literature review

Authorship and contributorship

This literature review is performed by the primary author, Zaman Sajid, under the guidance of Dr. Faisal Khan and Dr. Yan Zhang. Sajid collected and reviewed the literature and wrote the first draft. Co-authors Drs. Faisal Khan and Yan Zhang have reviewed the collected literature and also the first draft. They have provided feedback and revisions. Sajid has implemented these revisions and the latest version of the review is presented here.

2.1 Introduction

Generally, biodiesel process economics methods are based on process design and simulation, and provide an estimated cost of equipment, raw materials, operating costs, utility costs, overall cost of biodiesel production and the expected revenue from a biodiesel facility (Lim, Lee et al. 2009, Santana, Martins et al. 2010, Poddar, Jagannath et al. 2017). The high production cost of biodiesel from vegetable oils is a big hurdle in the commercialisation of biodiesel. The use of vegetable oils as food sources and the high cost of refined vegetable oil make vegetable oils an unfavourable biomass feedstock to produce biodiesel. Therefore, research is being focused to develop new raw materials and ways to minimize the cost of production (Gharat and Rathod 2013). Other raw materials include non-edible oils such as jatropha oil, low quality canola oil and palm oil. The use of these raw materials as biomass feedstock requires additional steps to extract their oils (Miller and Kumar 2014). Process economic studies are also being performed on the use of waste vegetable oil (WVO) biomass feedstock, since the cost of WVO is lower than the cost of using edible or non-edible oil (Glisic, Pajnik et al. 2016). Microalgae is also being considered as a potential feedstock to produce biodiesel, though production economics are a big challenge (Demirbas 2017). Moreover, the mathematical optimization models in finding the optimal (least cost and maximum profit) solutions and the cost reduction strategies are based on the cost and profit data being reported in these studies (Mohseni and Pishvaee 2016, de Jong, Hoefnagels et al. 2017). All these studies provide a conceptual "study estimate" of cost and revenue data for biodiesel production before the project is able to move into its design phase. Such estimates are typically used in early planning and initial feasibility studies to study return-on-investment (ROI) for a biodiesel investor. In a typical decision making process, if cost data prove to be too conservative, the project is not selected to move on to the next engineering stage. If this cost data is underestimated, the investors may experience substantial cost escalation from the initial estimated cost to the final construction cost of the plant (Gardner, Gransberg et al. 2016). Cost estimation accuracy is a major concern to other dimensions of engineering; it is reported that an uncertainty of -40% to +100% can be present in the estimated cost (AASHTO 2013), In process engineering, Turton and colleagues (2008) reported a range of +30% to -20% for expected accuracy. Hence, having relatively poor accuracy, the results of most biodiesel process economic studies may not accurately reflect the final cost and profitability of the chemical plant. Additionally, such studies do not show the level of risk associated with cost escalation. The estimation of biodiesel investment cost or capital cost is the very first step to determine the economic viability of a biodiesel project. For an innovative method to produce biodiesel, researchers perform labour-intensive work and predict the capital expenditure needed at an early stage of biodiesel product development. This information helps to assess alternative routes and identify a viable process to produce biodiesel. This step acts as a basis for the next step, which includes an iterative process to monitor the actual cost based on the initial cost estimate, once the project is approved and implemented (Gerrard 2000). However, if an initial estimate, being the basis for the next step, has uncertainty in its cost data, the cost at the biodiesel project execution stage could escalate, which may turn into a huge loss for a biodiesel investor. Moreover, in a recent work, Hollmann (Hollmann 2012, Hollmann 2012a) studied the accuracy of the estimated cost for more than 1,000 process industry projects, including oil and chemicals etc. The researcher reported that there was a cost overrun in 21% of the projects, while 10% of the projects even exceeded their estimated budgets by 70%. A biodiesel plant falls in the category of process plants similar to ones analysed by Hollmann, since a biodiesel plant employs unproven, innovative technologies for commercialization. Therefore, it is safe to assume that such a cost overrun could also occur in capital estimation of a biodiesel plant. Moreover, the capital cost of an industrial scale biodiesel plant is in billions of dollars; a discrepancy in cost estimation could lead to the financial disaster of the project.

2.2 Definition of terms

Before going into more detail in the literature review and defining the technical research gap, it is vital to describe some details of the concepts already well-established in the literature which are being used in this research work. This section highlights major concepts used in this thesis and their available techniques. The modifications in these existing techniques and applications of innovative techniques developed through this research work are presented in this thesis.

2.2.1 Value at Risk (VaR)

The measurement of risks associated with a portfolio is an essential task in financial engineering. In terms of market risks, this evaluation provides an estimation of potential losses which could likely occur when the price of a portfolio asset falls. In financial engineering and business economics, this risk measurement is called value at risk (VaR), which represents the maximum amount of money which an investor could lose from the return on investment with a given probability level and in a given time period (Abad, Benito et al. 2014). The VaR helps to study the impact of various market risk factors on a future portfolio and aggregates likely losses due to these risks into a single number (Zhou, Qin et al. 2016). This procedure develops an effective risk management tool for financial institutions or market investors. Owing to its conceptual simplicity, an ability to represent a risk profile in a single number, and accommodating the impact of different market risks, VaR is used by asset managers or traders extensively to assess the future market risks for financial assets such as bonds, stocks, or credit risk (credit VaR modelling). The VaR methodologies provide a recapitulative, conceptual, comprehensive and monetary based framework to measure market risks. Such market risks are depicted by the representation of the probability distribution of a random number and the risk is evaluated by analysing the probability distribution profile. Other than having applications in financial markets (Kellner and Rösch 2016), VaR has applications in analysing risks in the prices of energy commodities, (Hung, Lee et al. 2008), and crude oil markets risks (Lux, Segnon et al. 2016). The VaR characteristics are defined through three parameters which are: certainty level, time horizon over which analysis is made and the chosen calculus model (Tardivo 2002). There are three kinds of quantification methods for VaR (Sadeghi and Shavvalpour 2006): the historical method, variance-covariance method, and Monte Carlo Simulation.

1) Historical method

With the historical method, prior data to the time of calculation are used to develop an empirical distribution for the associated risk factors. This distribution is used to forecast future returns and provide VaR. The major advantage of this method lies in the fact that no assumption is made about the change in the distribution of the risk factors, and hence the changes in risk factors can be from any type of distribution.

However, the main disadvantage is that this method requires the availability of the risk data for a long historical period, which in many cases is hard to collect (Bohdalová 2007).

2) Variance-covariance method

In this method, potential losses and return standard deviations are directly proportional. In advanced models of Variance-covariance, past values and past deviations are combined to forecast future variance values. Though simple in calculation, this method has the disadvantage of being less efficient compared to the historical method (Sadeghi and Shavvalpour 2006).

3) Monte Carlo Simulation

In financial risk management, Monte Carlo simulation is the most powerful and flexible technique by far because it has the ability to consider all non-linearities and desirable distribution properties of a portfolio associated with various risk factors (Bohdalová 2007). Using this technique, a random number generator produces a large number (thousands or more) of hypothetical scenarios which are then used to develop a large number (thousands or more) of profit and loss events of the portfolio; subsequently, their arrangement generates the distribution of profit or loss. Finally, this distribution is used to determine VaR according to a required parameter (confidence level of 90%, 95%, or 99%) (Bohdalová 2007). In Chapter 5, this technique is explored to develop a methodology to compute VaR for a process facility.

2.3 Biodiesel process facility risks

Quite often biofuel policies are developed with inputs from scientists and research managers, government officials, particularly government policy-makers, and other public sector stakeholders (Levidow and Papaioannou 2013). An effective biofuel policy is only possible when there is a clear picture of how the key risks affecting the biofuel companies can be mitigated (Pries, Talebi et al. 2016). However, before such an effective means to mitigate risks are developed, managers, risk analysts, and investors first must understand the nature, categories, causes and conditions which develop such risks. Once the nature of such risks is identified then these risks should be taken into account while making an investment decision to build and develop new biofuel technology companies (Morrison, Witcover et al. 2016). Biodiesel performance risk analysis is a process to identify the potential threats to the performance of a biodiesel production plant, the analysis of the vulnerability to these threats and their preventive management to reduce the associated level of risk. In this management system, decision makers are risk averse and demand to have higher returns when engaging in risky activities such as commercialising new technologies of biodiesel production. In the literature, such risks are referred to as barriers, constraints or challenges (Blumer, Stauffacher et al. 2013), and are categorised as technical risks and non-technical risks. A detailed study of non-technical risk factors in the growth of the biofuel industry has been presented by Blumer and colleagues (2013) in their recent work. In their study, they identified five dimensions for non-technical risk factors for a biofuel industry. These were: project characteristics (size of a biodiesel plant etc.), policy framework, regional integration (availability of feedstock etc.), public perception (how the public will react to the use of biodiesel as an alternate fuel), and stakeholders. As is evident, non-technical risk factors affecting the performance of biodiesel have been well-addressed in the literature; however, the technical risks aspects of biodiesel performance have never been studied. In this thesis, these risk factors were classified based on three performance risk factors: process, design installation and operations. In Chapter 4, the nature of 57 different risk categories and different conditions of these risks are discussed. In a techno-economic performance measurement system, a study of the impact of such risk factors on biodiesel process economics is vital in biodiesel policy-making decisions. To date, there have been no such studies or techniques available in the literature. To address this issue, in Chapter 5, a concept of VaR is borrowed from financial engineering and introduced in a biodiesel process facility. A literature review reveals that this concept of VaR is being used in many other scientific dimensions. It was initially developed and used in stock markets and financial risk management, where VaR was typically used to determine the number of assets needed to cover the possible future losses or fluctuations in stock portfolios and bonds, in financial controlling, reporting, and computing regularity capital (Jorion 2006). Sanders and Manfredo (2002) introduced VaR in risk based decision making for a corporate purchasing department. More specifically, they implemented VaR on a publicly held food service company, which had exposure to market risks in food commodities. The portfolio they examined was based on the purchasing decisions of the essential inputs of a food service business, including soybean oil, wheat, boneless beef and raw coffee beans. They examined VaR based on a variance-covariance approach in which historical price fluctuation data were used to model future returns and the associated risk computation. They claimed that their analysis was applicable for any purchasing decisions or business that could be exposed to commodity price risks such as metals and energy.

In another application of VaR, Prettenthaler and colleagues (2016) utilized VaR to assess the effects of climate change. They studied the weather VaR, developed by

Toeglhofer and colleagues (2012), which studied the maximum expected loss due to adverse weather conditions for a given confidence level over a certain time period. They explained the concept of weather VaR using the cumulative distribution function (CDF) of a weather-dependent socio-economic indicator, in which the variability comes from the change in the weather conditions. They implemented their developed methodology on the agriculture and tourism sectors. The results of their study indicated that summer tourism in Sardinia has a higher increase in weather-induced income risks than does wheat cultivation in Cagliari.

Gokgoz & Atmaca (Gokgoz and Atmaca 2016) applied VaR to study the performance of the Turkish electricity market. They measured the portfolio performance and made a comparison of the approach with the traditional one, using the historical price data for two years, i.e., between April 2014 and April 2016. They adopted their data from the Turkish Day Ahead Market. Through the solutions of their optimization code developed in MATLAB, they identified that the performance measures through normal distribution assumption methods are superior in analysing system performance compared with the historical simulation based VaR. They also reported that in using historical VaR, the number of data and level of confidence integral play important parts in shaping the results. More data or a lower confidence integral in VaR computations provide more reliable and clear results.

Using the VaR analysis approach, Bianconi and Yoshino (Bianconi and Yoshino 2014) made an attempt to study risk factors and their impacts in the non-renewable energy sector. In their study, they collected the return on stock samples of 64 oil and gas companies from 24 countries from 2003 to 2012 and analysed VaR. In their econometric model, they measured the impact of systematic risk on the returns of oil and gas companies. Their results show that a naive calculation based on raw data over estimates the VaR, while VaR would be under estimated if calculations do not take into account the exposure.

McCormack and co-workers (2008) examined the integration of a supply-chain operations reference (SCOR) model with processes associated with potential risk elements in a supply chain's management. In doing so, they identified potential risk elements which assessed their impacts using various proposed techniques and risk matrix hierarchy levels. One of the techniques they presented was the application of VaR to evaluate and manage potential supply chain risks. They assessed supply chain risks from the prospective of the suppliers, the company and the consumer and presented the application of VaR on the supply chain by computing the highest likelihood of being late between Northwest and American airlines. With this example, they presented the performance based evaluation procedure for suppliers, customers (volume growth and profitability), and of products (guarantee claims). They also recommended using VaR to assess internal supply chain entities, which include distribution and manufacturing.

2.4 Integration of ISM and BN

Interpretive structural modelling is a methodology which identifies the relationships among different factors which define an issue or problem (Singh, Shankar et al. 2003). The nature of ISM analysis is qualitative one. Using ISM, various experts assess the pair-wise relation between risk factors and the data generated from these assessments is then used to develop a relation matrix which develops an ISM model (Shibin, Gunasekaran et al. 2016). The ISM model illustrates the hierarchy of the interdependency of various factors under study. This relationship pyramid is developed using the driving power and dependence power of each risk factor. The basic idea of ISM is to use experts' experience and knowledge to reduce a complex and complicated system to simple and well-defined sub-systems (elements). The multi-level structural model obtained as a result of ISM helps to understand complex situations and identifies a course of action by developing a map of complex relations among various factors to help resolve a problem. (Rade, Pharande et al. 2017). In developing the contextual relationship among variables, nominal group techniques, idea engineering and brainstorming techniques can also be utilized in combination with experts' opinions (Azevedo, Carvalho et al. 2013). A literature review revealed that the ISM technique is being used in different areas of study. Faisal and Talib (2016) applied ISM to understand the inter-relationships among different factors affecting the traceability in food-supply chains. As mentioned previously, one important aspect in ISM is the consultation with a group of experts. In their study, the group of experts consisted of professionals and management personnel working in the fields of food processing and academia. They chose a total of nine experts, consisting of six people from food industry and three from academia. Their study demonstrated that two factors, agro-terrorism threats and food safety, were the most important elements affecting the whole network of the food-supply chain. Ye and colleagues (2015) utilised the ISM technique to deal with the problem in the safety capacity of a petrochemical base and considered 14 factors that affect the safety capacity. In their study, experts were from companies and universities and the initial relationship between variables was developed after many rounds of discussion. They found that emergency rescue and safety management were the key variables affecting the safety capacity.

A Bayesian Network (BN) or belief network is a well-explained directed acyclic graph which encodes probabilistic relationships among different factors or nodes (circles) of interest in the problem (Pai, Kallepalli et al. 2003). A BN is the combination of graph theory and probability theory and enables the modelling of causal and probabilistic relationships in various types of decision-making processes (Zhou, Fenton et al. 2014). To represent a BN, a qualitative structure as well as a probabilistic relationship among the risk factors is needed. The qualitative structure helps to communicate inter-dependencies among risk factors in the form of a network, while the probabilistic relation defines the quantitative strength among these risk factors. BN is based on Bayes' theorem (Pai, Kallepalli et al. 2003) and is considered a special class of graphical model, which can be used to study causal dependencies between random variables. This means that in a directed edge (connecting line among nodes) from variable A to variable B in the model, new information in variable A would *cause* a change in the given information of B. In BN analysis, this new information is called *evidence* and variables A and B are called *parent* and *child* respectively. In the case of non-directed edges (variables A and B connected by a straight line with no arrow), no causal relationship in implied, but there is a correlation which represents a weak form of association. In this case, A and B are called *neighbours*. In the case of no edge (either directed or non-directed) between variables A and B, variables are said to be *independent*. In the case of a directed graph from A *to* B, a joint distribution is expressed as the product of P(A) and the probability of B given A or P(A)P(B/A) (Cowell, Verrall et al. 2007). BN uses directed acyclic graphs (DAG) which represent the conditional dependent relations among different and random nodes (variables) as shown in Figure 2.1, in which the numbers 1 to 10 depict the number of random variables or risk factors.

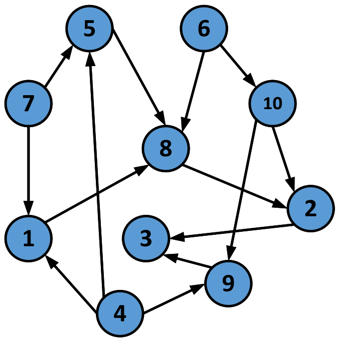


Figure 2.1 Directed acyclic graph (DAG)

The BN model is created by developing/assigning conditional probability tables (CPTs) to each node in a DAG. This step quantifies the strength of dependencies among nodes. BN has been successfully implemented on many real-world problems. Tang and colleagues (2016) studied the potential accident locations for water quality assurance using a BN approach. Their BN model identified the potential pollution risk and identified key factors including human factors. They defined risk in their study as risk of water pollution which could be caused by leakage of pollutants into fresh water. Out of nine major traffic accident factors, they identified human judgement and correct trucker response as the most sensitive variables in pollution accidents. Other research fields using BN include but are not limited to social science (Haapasaari and Karjalainen 2010), medicine (Forsberg, Eberhardt et al. 2011) and engineering (Langseth and Portinale 2007).

In most of the literature, either DAG is assumed or the variables are correlated through experts' judgment and brainstorming without following a proper scientific methodology (Helle, Ahtiainen et al. 2015; Tang, Yi et al. 2016; Rigosi, 2015). Since the results of the BN approach are based on DAG, a methodology to integrate a scientific way to correlate variables (such as an ISM model) and the BN approach can help to resolve this problem.

2.5 Biodiesel life cycle thinking

The life cycle thinking concept is widely accepted as a standard to assess the environmental impacts of products and services. This approach is based on the fact that many countries have adopted life cycle assessment in their regulations; for example, product certification in the British Standards Institute (BSI 2011), sustainability and biomaterials' certification from the Roundtable on Sustainable Biomaterials (RSB 2016), LCA regulations in the U.S Environmental Protection Agency (EPA 2010) and a European Parliament Directive (EU 2009). The results of LCA are also helpful in developing biodiesel policy and help biodiesel policy makers to analyse the environmental impacts of biodiesel throughout its life cycle (IEA 2010; Berndes 2011, Bird et al. 2011). Environmental life cycle analysis is a systematic tool which is used to assess the environmental impacts of biodiesel fuel throughout its life cycle. A life cycle of biodiesel fuel consists of the major stages: the use of raw materials (vegetable or non-vegetables crops), manufacturing, transportation of biodiesel to the market, distribution to the end user of biodiesel, disposal (combustion) and recycling (CO_2 released by biodiesel fuel absorbed by vegetable or non-vegetables crops) and then the use of these plants as raw materials (Malça, Coelho et al. 2014). The life cycle analysis stages of a typical product are shown in Figure 2.2.

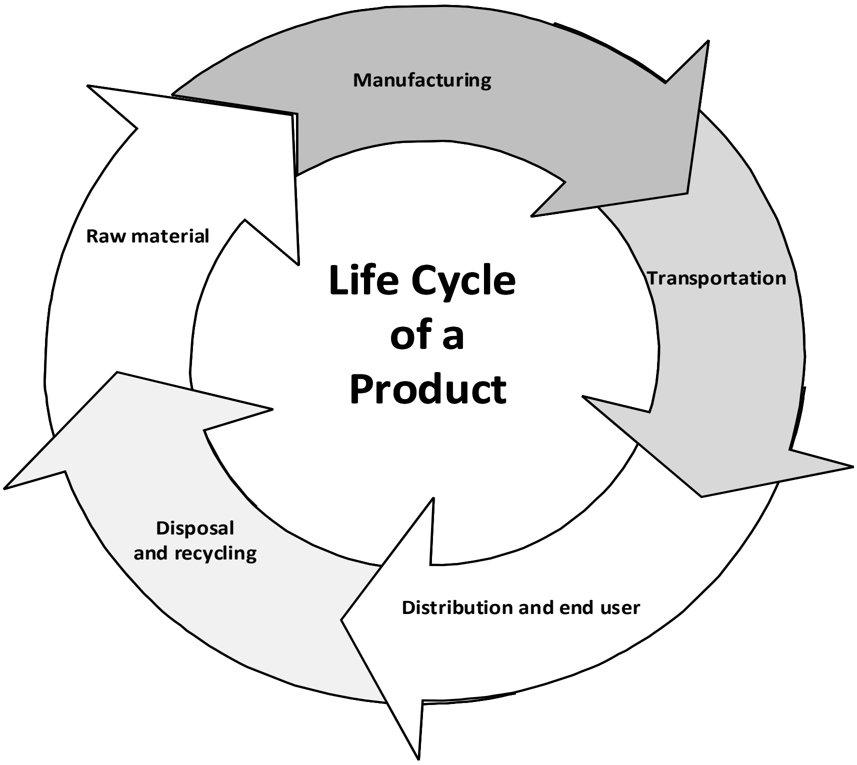


Figure 2.2 Environmental life cycle analysis stages

The combustion of biodiesel emits carbon dioxide, carbon monoxide, oxides of nitrogen, smoke and sulphur oxide. Using biodiesel as a combustion fuel, there is a 90% reduction in total unburned hydrocarbon (HC) and there is a 75-90% reduction in polycyclic aromatic hydrocarbons (PAHs). Moreover, the combustion of biodiesel yields less carbon monoxide and particulate matter compared to the combustion of petroleum based diesel fuel. However, based on the type of the engine, there seems to be a slight change in nitrogen oxides (Demirbas 2007).

Global warming is linked with the emissions of CO_2 into the atmosphere and therefore, to protect the environment, there is a need to control such emissions. Since biodiesel is produced from renewable sources, the use of biodiesel protects the environment and minimizes global air pollution. In particular, it helps to reduce emission levels of potential carcinogens (Canakci 2009, Ozsezen et al. 2009). In this regard, LCA techniques play a vital role to determine the quantitative environmental impacts of biodiesel, as demonstrated by various previous studies (Quinn and Davis 2015; Rajaeifar, Akram et al. 2016; Parajuli, Knudsen et al. 2017).

2.6 Technical and knowledge gaps

Research on biodiesel production, biodiesel chemical reaction chemistry and its use as an alternate fuel is well known; however, the research on biodiesel policy making when biodiesel is produced from wastes, performances of biodiesel production processes and risks in biodiesel process economics have not been closely assessed. Despite several extensive research studies, there remain many technological and knowledge gaps in addressing the economic and environmental sustainability of biodiesel. Therefore, this section attempts to highlight major technological and knowledge gaps that have not yet been addressed in the literature to date.

2.6.1 Technical gaps

Probabilistic economic risk analysis

As the literature review in Section 2.1 explains that the cost data in a biodiesel process economic study lack an adequate level of accuracy; consequently, there is a risk of cost escalation. Therefore, there is a need to develop a methodology for probabilistic economic risk analysis. This will help to mitigate the risk of cost escalation in performing biodiesel process economic analysis and will identify key elements causing cost ambiguity in the whole process. The analysis can help to make a biodiesel project an economical one and can save it from considerable financial disaster. This methodology has been presented in Chapter 3 of this thesis.

Interdependency model to measure biodiesel performance

As the literature review in Section 2.3 shows, there are various technical and non-technical risk factors which could affect the performance of a biodiesel plant. This identifies another significant gap to study these risks and in the analysis of their impacts on biodiesel performance. As presented in the literature review, many of these risk factors could be interdependent, so there is a need to develop an interdependency model to measure their combined effects on the performance of a biodiesel plant. This is achieved by developing a methodology integrating ISM and the BN approach. The robustness of the model comes from the fact that if the value of any risk factor is updated, the causal property of BN updates the whole network accordingly. In this way, the impact of one risk factor can be studied over the whole risk network or on individual risk factors in a quantitative way. The work is presented in Chapter 4 of this thesis.

VaR for biodiesel process applications

As is evident from the literature review in Section 2.3, VaR has been used in many arenas of science and engineering; however to date the technique has not been modelled for a process facility. To address this research gap, in Chapter 5, a new process-based VaR model is proposed that analyses the effects of different risk factors on biodiesel production profitability by considering their interdependent relationships, both qualitatively and quantitatively. The model helps to provide information about maximum possible loss with a certainty level over a given period. The results are helpful for process manufacturers, investors, managers and other stakeholders; as they identify bottlenecks in biodiesel processes and operations.

2.6.2 Knowledge gap

Some available studies and research works are lacking in scientific knowledge about the availability and resourcefulness of biomass feedstock. This also drives biodiesel policy makers towards an unclear path. The production of biofuels from first generation feedstock (food crops such as edible oil seeds, cereals and sugar crops) has exacerbated various challenges such as the rise in food prices, the use of land to grow crops and an increased life cycle carbon dioxide emission (Fargione, Hill et al. 2008, Sims, Mabee et al. 2010, Yang, Xu et al. 2011). To address these challenges, research moved to second generation biofuels, which included non-edible biomass feedstock such as grass, agriculture and forest residues, municipal solid wastes, waste oils, aquatic biomass etc. (Naik, Goud et al. 2010). Since the growth of non-edible crops still requires the use of land, researchers are focusing on third generation biofuels which include the use of algae as biomass feedstock (Lee and Lavoie 2013). In order to address the environmental impacts of biodiesel, develop guidelines for biodiesel policy making and biodiesel supply chain management, in Chapter 6, a detailed LCA study is performed using Jatropha oil – an inedible oil and waste cooking oil (WCO) as biomass feedstocks. Since these feedstocks are derived from different sources and different technologies are used to convert them into energy fuels, the requirements of energy and material are different in converting each feedstock into biodiesel (Kulkarni and Dalai 2006).

2.7 References

AASHTO (2013). Practical guide to cost estimating. Washington DC, American Association of State Highway and Transportation Officials (AASHTO).

Abad, P., S. Benito and C. López (2014). "A comprehensive review of Value at Risk methodologies." The Spanish Review of Financial Economics 12(1): 15-32.

Azevedo, S., H. Carvalho and V. Cruz-Machado (2013). "Using interpretive structural modelling to identify and rank performance measures: An application in the automotive supply chain." Baltic Journal of Management 8(2): 208-230.

Berndes, G., N. Bird and A. Cowie (2011). "Bioenergy, land use change and climate change mitigation." IEA Bioenergy retrieved from http://www.ieabioenergy.com/wp-content/uploads/2013/10/Bioenergy-Land-Use-Change-and-Climate-Change-Mitigation-Background-Technical-Report.pdf.

Bianconi, M. and J. A. Yoshino (2014). "Risk factors and value at risk in publicly traded companies of the nonrenewable energy sector." Energy Economics 45: 19-32.

Blumer, Y. B., M. Stauffacher, D. J. Lang, K. Hayashi and S. Uchida (2013). "Non-technical success factors for bioenergy projects-Learning from a multiple case study in Japan." Energy Policy 60: 386-395.

Bohdalová, M. (2007). "A comparison of value-at-risk methods for measurement of the financial risk." Faculty of Management, Comenius University, Bratislava, Slovakia.[Online], E-learning working paper,[Online] retrieved from https://www.g-casa.com/PDF/Bohdalova.pdf on Jan 24, 2017.

BSI (2011). Specification for the Assessment of The Life Cycle Greenhouse Gas Emissions of Goods and Services, British Standards Institution (BSI).

Canakci, M., A. N. Ozsezen, E. Arcaklioglu and A. Erdil (2009). "Prediction of performance and exhaust emissions of a diesel engine fueled with biodiesel produced from waste frying palm oil." Expert Systems with Applications 36(5): 9268-9280.

Cowell, R. G., R. J. Verrall and Y. Yoon (2007). "Modeling operational risk with Bayesian networks." Journal of Risk and Insurance 74(4): 795-827.

De Jong, S., R. Hoefnagels, E. Wetterlund, K. Pettersson, A. Faaij and M. Junginger (2017). "Cost optimization of biofuel production – The impact of scale, integration, transport and supply chain configurations." Applied Energy 195: 1055-1070.

Demirbas, A. (2007). "Importance of biodiesel as transportation fuel." Energy Policy 35(9): 4661-4670.

Demirbas, A. (2017). "Production economics of high-quality microalgae." Energy Sources, Part B: Economics, Planning, and Policy 12(5): 395-401.

EPA. (2010). "Renewable Fuel Standard Program (RFS2) regulatory impact analysis." Retrieved 16 April, 2017, from nepis.epa.gov/Exe/ZyPURL.cgi?Dockey=P1006DXP.TXT.

EU (2009). "Renewable Energy Directive 2009/28/EC." Official Journal of the European Union (EU): L.140/116 - L.140/162.

Faisal, M. N. and F. Talib (2016). "Implementing traceability in Indian food-supply chains: An interpretive structural modeling approach." Journal of Foodservice Business Research 19(2): 171-196.

Fargione, J., J. Hill, D. Tilman, S. Polasky and P. Hawthorne (2008). "Land clearing and the biofuel carbon debt." Science 319(5867): 1235-1238.

Forsberg, J. A., J. Eberhardt, P. J. Boland, R. Wedin and J. H. Healey (2011). "Estimating survival in patients with operable skeletal metastases: an application of a Bayesian belief network." PLoS One 6(5): e19956.

Gardner, B. J., D. D. Gransberg and J. A. Rueda (2016). "Stochastic Conceptual Cost Estimating of Highway Projects to Communicate Uncertainty Using Bootstrap Sampling." ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part A: Civil Engineering.

Gerrard, A. (2000). Guide to capital cost estimating, IchemE.

Gharat, N. and V. K. Rathod (2013). "Ultrasound assisted enzyme catalyzed transesterification of waste cooking oil with dimethyl carbonate." Ultrasonics Sonochemistry 20(3): 900-905.

Glisic, S. B., J. M. Pajnik and A. M. Orlović (2016). "Process and techno-economic analysis of green diesel production from waste vegetable oil and the comparison with ester type biodiesel production." Applied Energy 170: 176-185.

Gokgoz, F. and M. E. Atmaca (2016). "Financial Portfolio Optimization in Turkish Electricity Market via Value at Risk." World Academy of Science, Engineering and Technology, International Journal of Social, Behavioral, Educational, Economic, Business and Industrial Engineering 10(11): 3571-3581.

Haapasaari, P. and T. P. Karjalainen (2010). "Formalizing expert knowledge to compare alternative management plans: Sociological perspective to the future management of Baltic salmon stocks." Marine Policy 34(3): 477-486.

Helle, I., H. Ahtiainen, E. Luoma, M. Hänninen and S. Kuikka (2015). "A probabilistic approach for a cost-benefit analysis of oil spill management under uncertainty: A Bayesian network model for the Gulf of Finland." Journal of Environmental Management 158: 122-132.

Hollmann, J. K. (2012). "RISK. 1027 Estimate Accuracy: Dealing with Reality." AACE International Transactions, AACE International, Morgantown, WV, available at http://validest.com/index_htm_files/Hollmann_Accuracy.pdf

Hollmann, J. K. (2012a). "Estimate Accuracy: Dealing with Reality." Cost Engineering-Morgantown 54(6): 17.

Hung, J.-C., M.-C. Lee and H.-C. Liu (2008). "Estimation of value-at-risk for energy commodities via fat-tailed GARCH models." Energy Economics 30(3): 1173-1191.

IEA. (2010). "Sustainable Production of second-Generation Biofuels: Potential and perspectives in major economies and developing countries." Retrieved 16 April, 2017, from http://www.iea.org/publications/freepublications/publication/biofuels_exec_summary.pdf.

Jorion, P. (2006). Value at Risk, 3rd Ed.: The New Benchmark for Managing Financial Risk, McGraw-Hill Education.

Kellner, R. and D. Rösch (2016). "Quantifying market risk with Value-at-Risk or Expected Shortfall? – Consequences for capital requirements and model risk." Journal of Economic Dynamics and Control 68: 45-63.

Kulkarni, M. G. and A. K. Dalai (2006). "Waste cooking oil – An economical source for biodiesel: a review." Industrial & engineering chemistry research 45(9): 2901-2913.

Langseth, H. and L. Portinale (2007). "Bayesian networks in reliability." Reliability Engineering and System Safety 92(1): 92-108.

Lee, R. A. and J.-M. Lavoie (2013). "From first-to third-generation biofuels: Challenges of producing a commodity from a biomass of increasing complexity." Animal Frontiers 3(2): 6-11.

Levidow, L. and T. Papaioannou (2013). "State imaginaries of the public good: Shaping UK innovation priorities for bioenergy." Environmental Science and Policy 30: 36-49.

Lim, Y., H.-s. Lee, Y.-W. Lee and C. Han (2009). "Design and economic analysis of the process for biodiesel fuel production from transesterificated rapeseed oil using supercritical methanol." Industrial & Engineering Chemistry Research 48(11): 5370-5378.

Lux, T., M. Segnon and R. Gupta (2016). "Forecasting crude oil price volatility and value-at-risk: Evidence from historical and recent data." Energy Economics 56: 117-133.

Malça, J., A. Coelho and F. Freire (2014). "Environmental life-cycle assessment of rapeseed-based biodiesel: Alternative cultivation systems and locations." Applied Energy 114: 837-844.

McCormack, K., T. Wilkerson, D. Marrow, M. Davey, M. Shah and D. Yee (2008). "Managing risk in your organization with the SCOR methodology." The Supply Chain Council Risk Research Team: 1-32.

Miller, P. and A. Kumar (2014). "Techno-economic assessment of hydrogenation-derived renewable diesel production from canola and camelina." Sustainable Energy Technologies and Assessments 6: 105-115.

Mohseni, S. and M. S. Pishvaee (2016). "A robust programming approach towards design and optimization of microalgae-based biofuel supply chain." Computers & Industrial Engineering 100: 58-71.

Morrison, G. M., J. Witcover, N. C. Parker and L. Fulton (2016). "Three routes forward for biofuels: Incremental, leapfrog, and transitional." Energy Policy 88: 64-73.

Naik, S. N., V. V. Goud, P. K. Rout and A. K. Dalai (2010). "Production of first and second generation biofuels: a comprehensive review." Renewable and Sustainable Energy Reviews 14(2): 578-597.

Pai, R. R., V. R. Kallepalli, R. J. Caudill and M. Zhou (2003). Methods toward supply chain risk analysis. Systems, Man and Cybernetics, 2003. IEEE International Conference on, IEEE.

Parajuli, R., M. T. Knudsen, S. N. Djomo, A. Corona, M. Birkved and T. Dalgaard (2017). "Environmental life cycle assessment of producing willow, alfalfa and straw from spring barley as feedstocks for bioenergy or biorefinery systems." Science of The Total Environment 586: 226-240.

Poddar, T., A. Jagannath and A. Almansoori (2017). "Use of reactive distillation in biodiesel production: A simulation-based comparison of energy requirements and profitability indicators." Applied Energy 185, Part 2: 985-997.

Prettenthaler, F., J. Köberl and D. N. Bird (2016). "'Weather Value at Risk': A uniform approach to describe and compare sectoral income risks from climate change." Science of The Total Environment 543, Part B: 1010-1018.

Pries, F., A. Talebi, R. S. Schillo and M. A. Lemay (2016). "Risks affecting the biofuels industry: A US and Canadian company perspective." Energy Policy 97: 93-101.

Quinn, J. C. and R. Davis (2015). "The potentials and challenges of algae based biofuels: A review of the techno-economic, life cycle, and resource assessment modeling." Bioresource Technology 184: 444-452.

Rade, K. A., V. A. Pharande and D. R. Saini (2017). "Interpretive Structural Modeling (ISM) for Recovery of Heat Energy." International Journal of Theoretical and Applied Mechanics 12(1): 83-92.

Rajaeifar, M. A., A. Akram, B. Ghobadian, S. Rafiee, R. Heijungs and M. Tabatabaei (2016). "Environmental impact assessment of olive pomace oil biodiesel production and consumption: A comparative lifecycle assessment." Energy 106: 87-102.

RSB. (2016). "Roundtable on Sustainable Biomaterials (RSB)." Retrieved 16 April, 2017, from rsb.org.

Sadeghi, M. and S. Shavvalpour (2006). "Energy risk management and value at risk modeling." Energy Policy 34(18): 3367-3373.

Sanders, D. R. and M. R. Manfredo (2002). "The Role of Value-at-Risk in Purchasing: An Application to the Foodservice Industry." Journal of Supply Chain Management 38(1): 38-45.

Santana, G., P. Martins, N. d. L. Da Silva, C. Batistella, R. Maciel Filho and M. W. Maciel (2010). "Simulation and cost estimate for biodiesel production using castor oil." Chemical engineering research and design 88(5): 626-632.

Shibin, K. T., A. Gunasekaran, T. Papadopoulos, R. Dubey, M. Singh and S. F. Wamba (2016). "Enablers and Barriers of Flexible Green Supply Chain Management: A Total Interpretive Structural Modeling Approach." Global Journal of Flexible Systems Management 17(2): 171-188.

Sims, R. E., W. Mabee, J. N. Saddler and M. Taylor (2010). "An overview of second generation biofuel technologies." Bioresource technology 101(6): 1570-1580.

Singh, M., R. Shankar, R. Narain and A. Agarwal (2003). "An interpretive structural modeling of knowledge management in engineering industries." Journal of Advances in Management Research 1(1): 28-40.

Tang, C., Y. Yi, Z. Yang and J. Sun (2016). "Risk analysis of emergent water pollution accidents based on a Bayesian Network." Journal of Environmental Management 165: 199-205.

Tardivo, G. (2002). "Value at Risk (VaR): The new Benchmark for managing market risk." Journal of Financial Management & Analysis 15(1): 16.

Toeglhofer, C., R. Mestel and F. Prettenthaler (2012). "Weather value at risk: On the measurement of noncatastrophic weather risk." Weather, Climate, and Society 4(3): 190-199.

Turton, R., R. C. Bailie, W. B. Whiting and J. A. Shaeiwitz (2008). Analysis, synthesis and design of chemical processes, Pearson Education.

Yang, J., M. Xu, X. Zhang, Q. Hu, M. Sommerfeld and Y. Chen (2011). "Life-cycle analysis on biodiesel production from microalgae: water footprint and nutrients balance." Bioresource technology 102(1): 159-165.

Ye, J., Y. Sun and J. Xiao (2015). "System Impact Relation and Mechanism of Safety Capacity in Petrochemical Base." Open Petroleum Engineering Journal 8: 110-116.

Zhou, C., X. Qin, X. Diao and Y. He (2016). "Estimating multi-period Value at Risk of oil futures prices." Applied Economics 48(32): 2994-3004.

Zhou, Y., N. Fenton and M. Neil (2014). "Bayesian network approach to multinomial parameter learning using data and expert judgments." International Journal of Approximate Reasoning 55(5): 1252-1268.

Chapter 3

3 Process design and probabilistic economic risk analysis of bio-diesel production

Authorship and contributorship

This work has been published by Sajid, Z., Zhang, Y., & Khan, F. (2016). “Process design and probabilistic economic risk analysis of bio-diesel production”. *Sustainable Production and Consumption*, 5, 1-15. It can be accessed at the link:

http://www.sciencedirect.com/science/article/pii/S235255091500038X

The co-author, Dr. Faisal Khan, identified the initial research problem. The first author, Zaman Sajid, developed the research methodology, performed the analysis, conducted the case study and drafted the manuscript. The co-authors, Drs. Yan Zhang and Faisal Khan, supervised this work at all stages from methodology development to the submission of the manuscript. Co-authors reviewed the research results, provided detailed comments and also reviewed the manuscript and provided constructive feedback. The first author, Zaman Sajid, has implemented feedback from co-authors and also from the peer reviewers.

Abstract

Process design and economic risk analysis was performed for a biodiesel production plant having an annual production capacity of 45,000 t of biodiesel using inedible Jatropha oil as the biomass feedstock. Five major economic factors associated with the cost were computed and analysed. These included total capital investment, fixed cost, variable cost, annual operating cost and total cost. Probabilistic cost estimation was performed to analyse the variability in the cost data. Among all other cost elements, raw material cost was found to be the most significant variable affecting the economic viability of biodiesel production system. Probabilistic risk estimation showed that, even using the published cost data, the estimated total risk was 50% uncertain. The study also showed that by incorporating environmental benefits of biodiesel burning, the benefit to risk ratio increased.

3.1 Introduction

Biodiesel is an environmentally friendly biofuel for diesel engines and is an alternative to conventional petroleum based diesel fuels. On a large industrial scale, it is produced by a chemical reaction of feedstock (edible vegetable oil or inedible oils or animal fats) with an alcohol (methanol or ethanol) in the presence of a catalyst (alkaline, acidic or enzymatic). The reaction is called trans-esterification. Stoichiometrically, one mole of triglyceride (feedstock) reacts with three moles of methanol (alcohol) to form three moles of fatty acid methyl ester (FAME), known as biodiesel. The reaction produces glycerol, which is generally considered a by-product of a trans-esterification reaction. The process of biodiesel production has much been studied by various researchers (Kumar, Ravi, & Chadha, 2011; Hawash, Diwani, & Kader, 2011; Raja, Smart, & Lee, 2011; Banković-Ilić, Stamenković, & Veljković, 2012).

Currently, the high cost of biodiesel production remains a big hurdle to its large-scale commercialization. Therefore, the economic assessment of biodiesel production has been a central focus of recent research. Various economic studies of biodiesel production have been performed using different technologies, raw materials and production capacities (Zhang Y. , Dube, McLean, & Kates, 2003a; West, Posarac, & Ellis, 2008; Cynthia & Teong, 2011).

Zhang et al. (2003b) assessed the economics of four different biodiesel plants using different raw materials. Haas et al. (2006) developed a computer model to estimate operational and capital cost of a biodiesel production facility. Kasteren and Nisworo (2007) studied the economics of biodiesel production at three plants operating at different capacities. You et al. (2008) reported the economic analysis of biodiesel production using soybean oil as raw material. Lopes et al. (2013) performed the economic feasibility of biodiesel using Macauba oil as raw material in Brazil. Nagarajana et al. (2013) studied the cost of biodiesel production using algae as a raw material. Most of these studies used the static cost data published on web-sites or by government departments.

Previous economic assessments of biodiesel production were based on cost data reported in open literature. None explain how reliable their cost data are and how much uncertainty is present in their cost data. The uncertainty present in the cost data greatly influences the accuracy of the total cost of biodiesel production. A few researchers have reported that the accuracy of their cost estimation was within a range of +30% to -20% (Zhang Y. , Dube, McLean, & Kates, 2003b; West, Posarac, & Ellis, 2008). Since their estimated cost is millions of dollars and may be even 1% uncertainty in it, the actual cost may exceed the expected cost value. This may result in a huge cost escalation and the project may become uneconomical. Moreover, their project profitability criteria do not account for uncertainties present in estimated cost data. The presence of uncertainty in the cost data significantly affects the accuracy of the results of economic analysis. Generally, there are uncertainties present in both the estimated cost and the estimated revenue data. Therefore, it is important to include a probabilistic analysis in any techno-economic study of biodiesel processes.

The present study performs an economic analysis of a biodiesel plant with an annual production capacity of 45,000 t of biodiesel from Jatropha oil using a homogeneous base catalysed process. This work develops a risk analysis methodology and the technique developed is demonstrated on a biodiesel case. This study deals with the uncertainties present in the estimated cost and the estimated revenue. A probabilistic cost-benefit analysis is also conducted to address the potential economic risk and the results provide an accurate indication of the return period over the period of investment.

3.2 Probabilistic Economic Risk Analysis Methodology

3.2.1 Basis and scope of calculations

The economic as well as probabilistic economic analyses were based on the following assumptions. (1) The process is based on a production capacity of 45,000 t/yr biodiesel. (2) Including the maintenance and breakdown schedules, the plant operates 8000 h/year. (3) The cost of oil includes the cost of extracting the oil from Jatropha *curcas* seeds and the oil does not contain any impurities and is free from water content. (4) All costs, revenue and profit data are shown in US $ and the respective values are valid for the year 2013. One Australian dollar is taken as equivalent to US $0.94. The prices of the equipment were updated to year 2013 from year 2001 using Chemical Engineering Plant Cost Index (CEPCI, 2014). The index for year 2001 was 394.3 and for year 2013 was 567.3. (5) The asset depreciation and plant decommissioning are not considered in this analysis. (6) The prices of biodiesel and other products are retail prices. Both the prices of biodiesel and mineral diesel exclude transportation, excise tax and distribution cost. (7) Only positive percentile values are studied for probabilistic analysis. (8) Being less in cost value as compared to the rest of the equipment, the equipment risk analysis ignores the probabilistic curves for the splitter (S-206), gravity settler (S-202) and liquid-liquid extraction unit (S-204).

3.2.2 Methodology Description

The methodology to perform this research is divided into two major steps.

1. *Process description and economic analysis:* The process flow diagram (PFD) for biodiesel manufacturing was selected and the fundamental material and energy balances were performed on a Microsoft Excel sheet. Process design was carried out using Aspen HYSYS version 7.3. The results of equipment sizes obtained from process design were used to estimate the capital costs and annual operating costs.
2. *Probabilistic risk analysis:* This step included the probabilistic risk analysis and the probabilistic cost-benefit analysis. Vagueness in cost and revenue of biodiesel production system were also incorporated into the study. The probabilistic cost-benefits analysis was conducted with and without the time domain. The methodology for the current research is sketched in Figure 3.1.

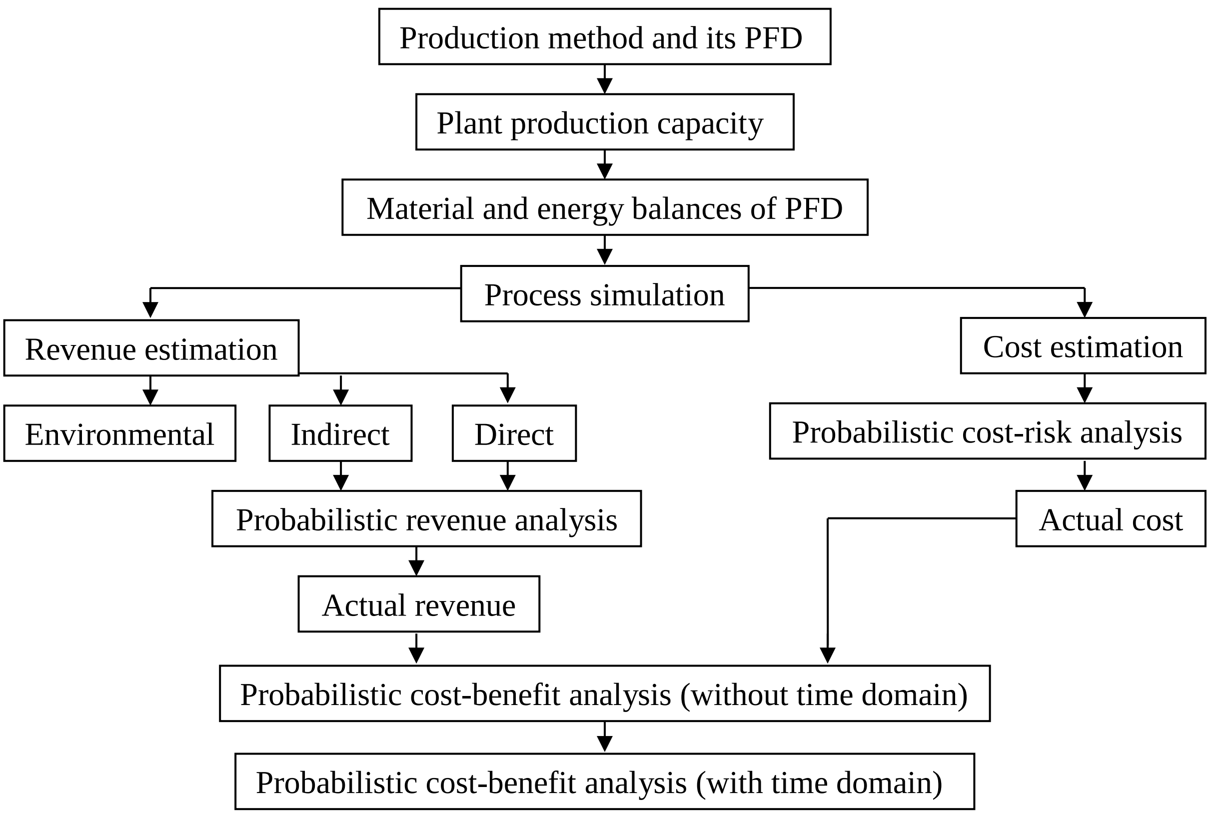


Figure 3.1 Methodology for probabilistic economic risk analysis

3.2.2.1 Process description

The biodiesel production process, its reaction kinetics and the latest conversion techniques from different raw materials have already been much defined (Zhang Y. , Dube, McLean, & Kates, 2003a; West, Posarac, & Ellis, 2008; Myint & El-Halwagi, 2009; Keera, Sabagh, & Taman, 2011; Nasir, Daud, Kamarudin, & Yaakob, 2013; Yusuf & Kamarudin, 2013). The alkali-catalysed biodiesel process was chosen to perform economic analysis. The raw material for producing biodiesel was Jatropha oil obtained from Jatropha *curcas* seeds. Jatropha oil is inedible and does not require any special kind of soil to grow its seeds. Moreover, it eliminates the debate between food resources and fuel for energy (Balat, 2011). The PFD of the biodiesel production process from Jatropha oil, shown in Figure 3.2, was adopted from literature (Rahman, Mashud, Roknuzzaman, & Al Galib, 2010; Abbaszaadeh, Ghobadian, Omidkhah, & Najafi, 2012). Chemical and physical properties of Jatropha oil and its FAME were extracted from literature (Kywe & Oo, 2009).

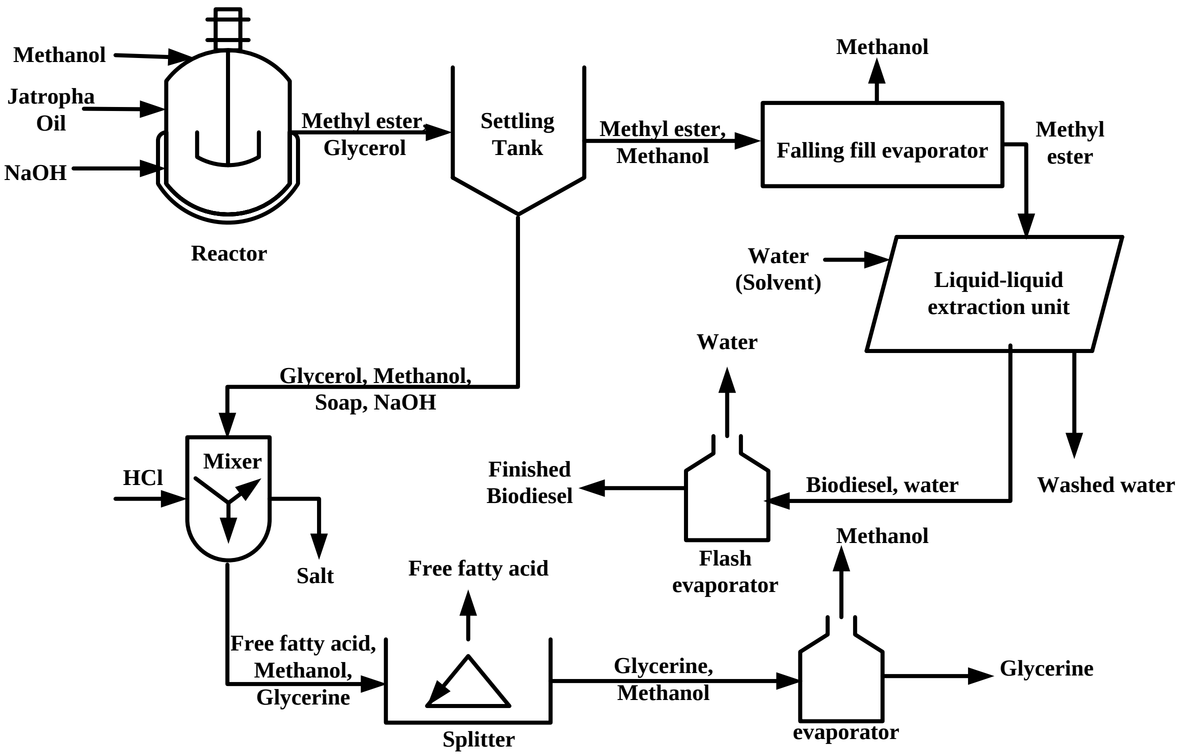


Figure 3.2 Process flow diagram (PFD) for biodiesel production

3.2.2.2 Process Simulation and Sizing

Before proceeding to the HYSYS simulation step, the following assumptions were made regarding different process parameters:

- Perfect mixing in the reactor was assumed.
- For the gravity settler, the separation efficiency was assumed to be 80%.
- The main reaction conversion was 95%.
- The reference temperature for energy balance was 25 °C.

The method for process simulation involved describing the chemical components, choosing the proper system of units, defining the stream conditions (temperature, pressure, flow rate, compositions of components in a stream) and selecting an appropriate thermodynamic model. Most of the components under study such as glycerol, methanol, hydrochloric acid, water and sodium hydroxide were available in the HYSYS library. Jatropha oil and its FAME were not present in the HYSYS library. Triolein ($C_{57}H_{104}O_6$) and methyl oleate ($C_{19}H_{36}O_2$) in Jatropha oil and its FAME had been chosen in previous research studies (Yusuf & Kamarudin, 2013) were used to represent Jatropha oil and its biodiesel in this study. The properties of methyl ester (methyl oleate) were present in the HYSYS component library. Triolein was defined in HYSYS using a 'hypo manager' tool. The enthalpies of the formation of oil and its respective methyl ester were taken from literature (Borghi, Abreu, & Guirardello, 2012; Lapuerta, Rodriguez-Fernandez, & Oliva, 2010). Since there were highly polar components (glycerol and methanol) present in the system, the activity coefficients of the components were estimated using a universal quasi-chemical (UNIQUAC) model (Zhang Y. , Dube, McLean, & Kates, 2003a; Kasteren & Nisworo, 2007). Material and energy balances for the entire biodiesel production were carried out on a Microsoft Excel spreadsheet (Himmelblau & Riggs, 2012). The results of the spreadsheet were used to perform the process simulation in HYSYS and the simulation results defined the sizes of the process equipment.

3.3 Economic Analysis Methodology

3.3.1 Cost estimation

In the current study, economic analysis refers to the estimation of fixed capital, working capital, project total investment and the annual operating costs. The annual operating costs include annual variable cost and fixed cost. Fixed capital cost refers to the construction cost of a new plant, which includes the cost to purchase equipment, equipment erection cost, building cost and the site development cost. The working capital cost represents operating liquidity available to the operation and the organization of the entire process facility. According to Sinnott (2005), the working capital is considered as 10% of the fixed capital. Variable cost, varying from the production level, includes the costs of raw materials, catalysts and utilities. The fixed cost, consisting of supervision charges, insurance, plant overhead and various other fixed charges is also needed to operate the plant. Direct production cost is the sum of variable and fixed costs. Annual operating cost includes direct production costs, sales expenses and research and development costs.

In the present study, the factorial method of cost estimation was used to find all the economic parameters listed above (Sinnott, 2005). The method was based on finding the total purchase cost of major equipment (PCE) in a process flow diagram used to produce biodiesel. All direct or indirect plant costs were functions of major equipment costs. The results of HYSYS sizing were used to estimate the major equipment costs. Equipment and utilities costs were adopted from literature (Peters, Timmerhaus, & West, 2002; Ulrich & Vasudevan, 2004).

The cost of Jatropha oil and other chemicals was adopted from Cynthia and Teong (Cynthia & Teong, 2011) and Chemical Business (Chemical Business, 2013) respectively. Where necessary, the cost data were updated to the year 2013 using the cost index. A spread sheet was prepared for the purchase cost of major equipment, fixed capital, working capital and the operating cost. The start-up schedule for a biodiesel plant was adopted from Towler and Sinnott (2012a). It was assumed that the plant was built with 30% of fixed capital cost in year 0 and that the rest of the fixed capital cost was utilized in year 1. The plant started to produce biodiesel in year 2. The plant operated at 50% of its full capacity in this year. This utilized a 50% variable production cost in year 2 and a 100% fixed production cost. Since the plant was operational in year 2, 100% of the working capital was utilized then. In subsequent years, year 3, year 4 and year 5, the plant produced biodiesel at its full capacity and both the variable production cost and fixed production cost were fully utilized. Towler and Sinnott provide an Excel sheet for this economic analysis, showing the production schedule (Towler & Sinnott, Excel Templates, 2012b).

3.3.2 Revenue estimation

The revenue from biodiesel production plant was divided into three categories.

1. Direct revenue

Direct revenue was the revenue obtained by selling the biodiesel. The average selling price of biodiesel was $4.43/gallon (US) (Energy, 2013). The reported average selling price was an average value of biodiesel prices taken at 55 different points across the United States. The profit for unit gallon of biodiesel produced was estimated by subtracting the estimated unit cost from the selling price of biodiesel.

2. Indirect revenue

Indirect revenue refers to the revenue generated by selling the by-products produced in the production of biodiesel. These by-products were glycerol, free fatty acid, and sodium chloride salt. The selling prices for these by-products were taken from the literature. Average prices of glycerol (glycerine), free fatty acid and salt were $1.29/kg (You, et al., 2008), $1.58/kg and $0.085/kg (Chemical Business, 2013) respectively. Where necessary, the prices were updated to the year 2013 using the cost index.

3. Environmental benefits

Biodiesel is an environmentally friendly fuel. Because biomass and biomass-derived materials are carbon neutral, the amount of carbon dioxide absorbed by crops during their growth balances that produced by combustion of biodiesel prepared from those crops. However, one cannot justify the use of biodiesel as carbon neutral only on this basis. Since there is a major debate on the land used to grow crops, as discussed by the International Panel on Climate Change (IPCC) (Ciais, et al., 2013). In the current study, 'environmental benefits' were the monetary advantage obtained by the combustion of biodiesel instead of diesel. This monetary advantage could be based on either unit of energy contents of the respective fuels, or unit mass of respective fuels. Since the current study is dealing with production quantities, therefore, burning of unit mass of the respective fuels is taken into consideration. The monetary advantage was obtained by considering the amount of carbon present in the unit mass of mineral diesel and biodiesel (Kalnes, Marker, & Shonnard, 2007). The amount of carbon was converted into dollar value using the carbon tax reported for the year 2013-2014 by the Clean Energy Regulator (Clean Energy, 2012).

The total revenue was the sum of revenue earned from direct revenue, indirect revenue and the environmental benefits. According to the previously mentioned plant start-up schedule, the plant was operational in year 2; hence, there would be no revenue for year 0 and year 1. In year 2, the plant was operating at 50% of its capacity, therefore, total revenue in year 2 was 50% of the total revenue and in the subsequent years, the plant would yield full revenue, as it would be operating at its full capacity.

3.3.3 Cost-Benefit Analysis

Cost benefit (benefit-cost) ratio analysis (CBA) is a technique use to evaluate the project's ability to make a profit. The benefit-to-cost ratio is represented as B/C in this study, where benefits (B) refer to the net profit i.e., total revenue minus total costs and the cost (C) represent the total cost of producing biodiesel. During the plant's construction, the total cost would be the sum of the fixed capital and working capital used in that year. Benefits and costs are estimated on annual basis. The profitability criterion is defined as follows: a project is acceptable if the B/C ratio exceeds zero. The benefit-to-cost ratio or (revenue –cost)/cost can be as low as -1 (i.e., revenue is zero).

3.4 Probabilistic Risk Analysis

Due to uncertainty in the form of variability in the input data and vagueness associated with operations, design and the cost estimation, a detailed probabilistic risk analysis was conducted. The probabilistic risk analysis methodology was developed to find, first, the risk associated with the total cost of biodiesel production, followed by the risk associated with the revenue estimations. Then, the methodology was implemented to find the risk involved in the cost estimation of major equipment used to produce biodiesel. As a criterion to evaluate the project profitability, a probabilistic cost-benefit analysis was performed. In this context, risk was defined as the likelihood of not meeting the defined target. In the case of cost estimation, the risk was the likelihood of the cost being greater than estimated. In the case of revenue estimation, the risk was the likelihood of having the revenue less than estimated.

3.4.1 Probabilistic cost risk analysis and cost-benefit analysis

Probabilistic cost risk analysis includes the vagueness associated with cost. It is differentiated from simple cost analysis by the fact that in cost analysis, the cost data is represented without including vagueness. The first approach to economic risk analysis in agricultural investment decisions was developed by Richardson and Mapp

(1976) and has been cited by various researchers (Richardson, Herbst, Outlaw, & Gill II, 2007; Yeboah, Naanwaab, Yeboah, Owens, & Bynum, 2013). Their methodology consisted of developing the cumulative probability distribution of Net Present Value (NPV) on investment and analysing the profile at the required level of risk probability. Cash flow over the life of the project was accounted for by simulating the cash flow for each year of investment made. This methodology was modified to implement the current study by considering the following variations:

1. The critical variable used in the simulation studies was Net Present Value (NPV). The critical variable in the current simulation was the cost, since the objective of current research was to perform risk analysis on cost data. For the time-domain study of cost, the time value of money was utilized and the cost data was updated to the next year's cost data using annual interest rates and inflation rates.
2. In their study, the minimum and maximum values for probability distributions of each variable were assigned with the help of experts. In the current study, these values were assigned within 10% of their most likely values.

The risk in the case of cost estimation has been defined in the previous section. Mathematically, the risk associated with cost is:

Risk = $P*C$

where P is the probability of not meeting the defined cost target and C shows the cost associated with the target.

The methodology to perform the current economic risk analysis on the total cost is shown in Figure 3.3.

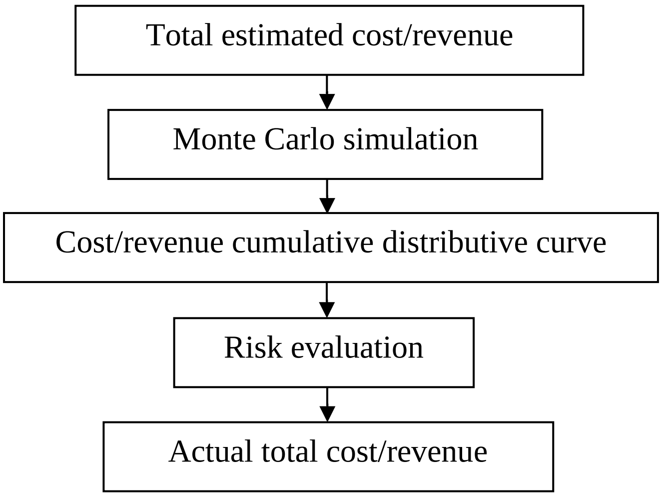


Figure 3.3 Economic risk analysis

Oracle® Crystal Ball software was utilized to perform a Monte Carlo simulation on the total production cost data. The total estimated cost was updated using the annual interest rate and inflation rate. The cumulative distributive curves obtained from the simulation were used to assess the risk associated. The actual total cost was calculated using the following equation:

Actual total cost = Estimated total cost + Cost risk

Since the actual total cost included the risk of exceeding the estimated cost value, a cost-benefit analysis was performed to evaluate the project profitability under these circumstances. Benefit to cost ratios were performed for estimated costs and actual costs on an annual basis and the results were compared.

3.4.2 Probabilistic revenue risk analysis and cost-benefit analysis

The revenue was estimated using the selling price of each individual product produced. Most often variability exists in the selling price data; it is therefore important to assess the probabilistic risk analysis for revenue data. To perform the probabilistic risk analysis on revenue, it was assumed that the revenue in the study would be the sum of direct and indirect revenues only and for current probabilistic analysis the environmental benefits were not considered. A Monte Carlo simulation was performed on the revenue data and the risk of having revenue lower than estimated was reported using the revenue cumulative probability plots. The actual revenue was calculated by subtracting the revenue risk from the estimated revenue. The procedure was repeated for the next year's revenue by updating the revenue in the time-domain as explained in the probabilistic cost risk analysis. Figure 3.3 shows the method developed for probabilistic risk revenue analysis.

Risk for revenue is defined as the likelihood of not meeting the defined revenue. Mathematically,

Risk = $P*R$

where P is the probability of not meeting the defined revenue target; R is revenue associated with the target. As the uncertainty in revenue leads to uncertainty in project profit, it is essential to re-examine the probabilistic cost-benefit analysis and the probabilistic revenue risk analysis.

3.4.3 Probabilistic risk analysis on major equipment of PFD

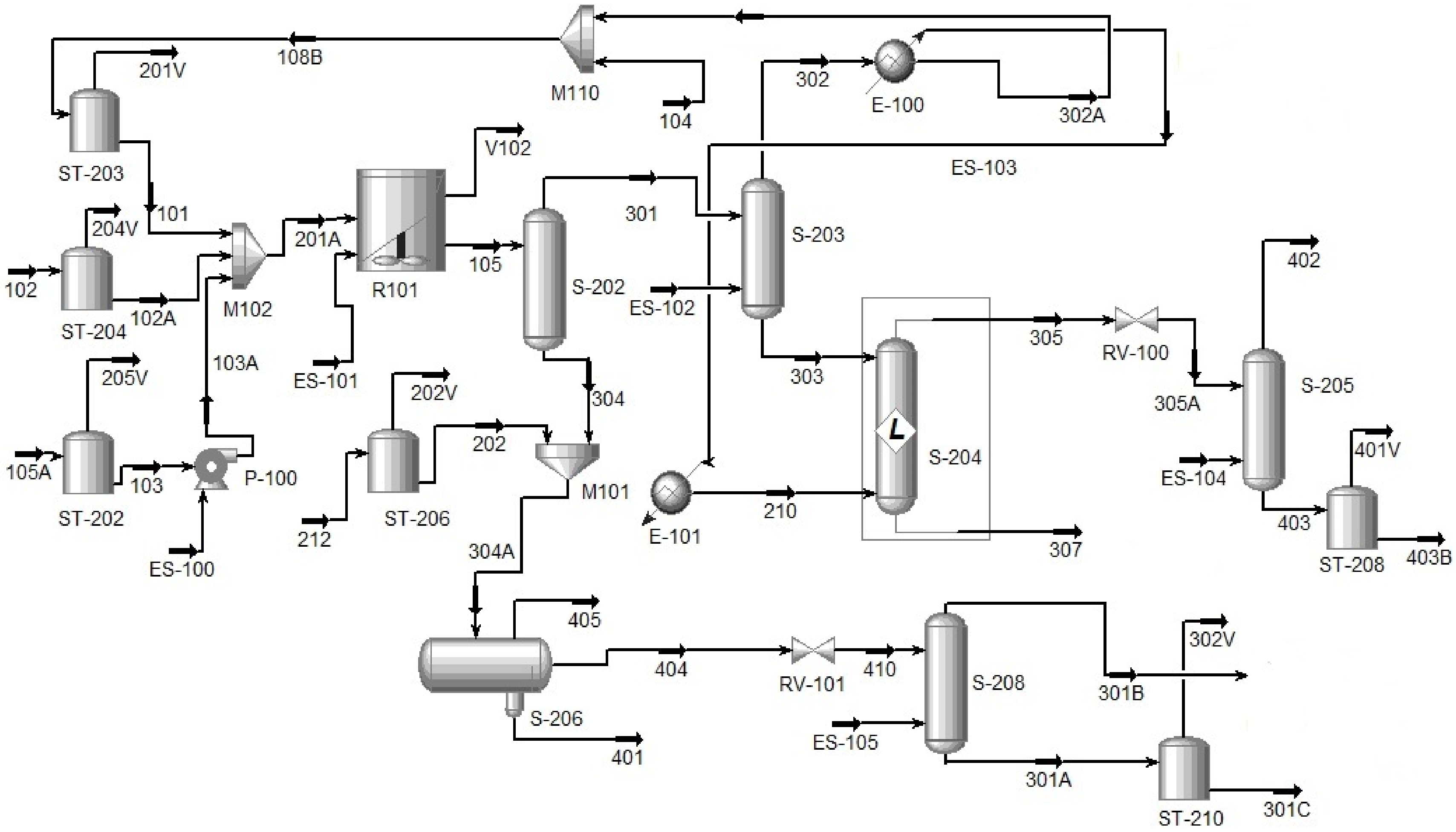
The analysis of the methodology used to estimate total production cost reveals that the cost of a single piece of equipment used to produce biodiesel has a great impact on the total production cost. Hence, the variability present in the cost of equipment alone could affect the process economic analysis significantly. Therefore, risk analysis on the cost of each piece of equipment is necessary. This type of study would help the decision maker to determine which equipment could have more cost risk and which equipment is contributing more or less to make the project an economical one. The methodology to perform risk analysis on production equipment was similar to the one used to analyse risk in the total cost, with the difference that a Monte Carlo simulation was performed on the estimated cost of all equipment. The cumulative distributive curves for equipment were used to analyse the risk of exceeding the targeted cost. The actual cost of important equipment was calculated as illustrated below:

Actual cost of equipment = estimated cost of equipment + equipment cost risk

3.5 Results and Discussion

3.5.1 Process Simulation and Economic Analysis

For an annual production capacity of 45,000 t of biodiesel, the HYSYS equipment sizing results and their respective estimated costs are obtained. The HYSYS simulation model is shown in Figure 3.4 and stream properties in Table 3.1. Table 3.2 shows the equipment sizing and the estimated purchase cost of major equipment used to produce biodiesel. Utilizing the total cost of major equipment, the results of estimated fixed capital, working capital and total capital investment are shown in Table 3.3. Table 3.4 presents the estimated variable and fixed cost needed to produce biodiesel on an annual basis.



Legend: R (reactor), ST (storage tank), M (mixer), P (pump), S (separating unit), E (heat exchanger), L (liquid-liquid extraction unit)

Figure 3.4 HYSYS simulation model to produce biodiesel from Jatropha oil using alkali-catalysed process

Table 3.1 HYSYS simulation stream properties

Stream Number	Molar flow (kmol/h)	Component mole fraction Methanol	Oil	FAME (Biodiesel)	NaOH	FFA	NaCl	HCl	Soap	Water	Glycerol
102	1.68	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000
202	2.43	0.000	0.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000
301	21.59	0.111	0.001	0.869	0.006	0.000	0.000	0.000	0.001	0.010	0.002
302	0.60	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
304	10.67	0.022	0.000	0.000	0.187	0.000	0.000	0.000	0.086	0.000	0.705
305	32.59	0.003	0.000	0.843	0.000	0.000	0.000	0.000	0.000	0.153	0.000
401	2.50	0.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000
405	1.83	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000	0.000
105A	6.22	0.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
301B	0.18	0.363	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.637	0.000
301C	6.29	0.100	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.050	0.850
403B	20.83	0.000	0.000	0.996	0.000	0.000	0.000	0.000	0.000	0.004	0.000

Table 3.2 Process Sizing

Process equipment	Tag	Description	Specification	Cost (US $ millions)
Reactor	R101	Temperature, ^oC	60	0.154
		Pressure, kPa	400	
		Size (D × H), m	3.2 × 9.6	
		Type	Cylindrical	
		Orientation	Vertical	
Separation unit	S-202	Temperature, ^oC	60	0.014
		Pressure, kPa	101.3	
		Size (D × L), m	1.06 × 17.78	
		Boot specs: D × H, m	0.68 × 1.02	
		Orientation	Vertical	
	S-203	Temperature, ^oC	75	0.092
		Pressure, kPa	101.3	
		Size (D × H), m	1.50 × 2.25	
		Reboiler duty, MJ	440.62	
		Condenser duty, MJ	96.95	
		Type	Falling film	
	S-204	Temperature, ^oC	50	0.082
		Pressure, kPa	101.3	
		Stages	8	
		Tray diameter, m	1.43	
		Weir dimension (H × L), m	0.16 × 1.2	
		Tray space, m	0.5	
		Tray volume, m3	0.88	
	S-205	Temperature, ^oC	98	0.097
		Pressure, kPa	94.3	
		Size (D × H), m^2	76.02	
		Reboiler duty, MJ	281.7	

	S-206	Temperature, ^{o}C	60	0.011
		Size (D × L), m	1.42 × 17.78	
		Boot specs (D × H), m	0.50 × 0.75	
		Orientation	Horizontal	
	S-208	Temperature, ^{o}C	75	0.087
		Pressure, kPa	94.3	
		Size (D × H), m	1.36 × 2.052	
Storage tank	ST-202	Capacity, m^3	1033	0.108
	ST-203	Capacity, m^3	128.79	0.043
	ST-204	Capacity, m^3	9.072	0.010
	ST-206	Capacity, m^3	12.53	0.013
	ST-208	Capacity, m^3	52.94	0.030
	ST-210	Capacity, m^3	1.381	0.004
Neutralizer	M101	Temperature, ^{o}C	60	0.025
		Pressure, kPa	101.3	
		Size (D × H), m	0.533 × 1.77	
			Total equipment cost	0.770

Table 3.3 Capital cost

Item	Cost (US $million)
Purchase Cost of major Equipment (PCE)	0.770
Fixed Capital Cost (FCC) = $I_{fraction}$ × PCE	
Equipment erection (0.4)	0.308
Piping (0.7)	0.539
Instrumentation (0.2)	0.154
Electrical (0.1)	0.077
Building process (0.15)	0.115
Utilities (0.5)	0.385
Storage (0.15)	0.115

Site development (0.05)	0.038
Ancillary building (0.15)	0.115
Subtotal, Physical Plant Cost (PPC)	2.618
Design and engineering (0.3)	-
Contractor's fee (0.05)	-
Contingency (0.1)	-
Plant Fixed Capital (PFC) = PPC* (1+0.3+0.05+0.1)	3.793
Plant Working Capital (PWC) = 10% of PFC	0.379
Total Capital Investment (TCI) = PFC +PWC	4.172

Table 3.4 Operational cost

Item	Cost (US $million)
Variable cost	
Raw material cost, $/t	
Jatropha Oil, 98.90	4.703
Methanol, 653.25	3.450
Sodium hydroxide, 774.3	0.693
Hydrochloric acid, 104.06	0.348
Subtotal, raw material	9.194
Miscellaneous materials (10% of maintenance cost)	0.037
Utilities cost	
Steam, ($1.65/1000 kg)	0.253
Process water, ($0.073/ m^3)	0.004
Cooling water, ($0.013/ m^3)	0.001
Natural gas, ($0.022/ m^3)	0.025
Subtotal, utilities	0.283
Shipping and packaging	1.500
Total variable cost (VC)	11.02
Fixed cost	

Maintenance, 10% of fixed capital	0.379
Operating labour	4.238
Laboratory cost, 20% of operating labour	0.848
Supervision, 20% of operating labour	0.848
Plant overhead, 50% of operating labour	2.119
Capital charges, 15% of fixed capital	0.570
Insurance, 1% of fixed capital	0.038
Local taxes, 2% of fixed capital	0.076
Royalties, 1% of fixed capital	0.038
Total fixed cost (FC)	9.15
Direct production cost (C), C = VC + FC	20.17
Sales expense, general overheads, company miscellaneous, research & development, employee development funds (D)	9.030
Annual Operating Cost (AOC) = C + D	29.20
Total Cost (TC) = AOC + TCI	33.38

According to the plant start-up schedule, the estimated cost for years 0, 1, 2, 3, 4, 5 is \$1.96, \$2.93, \$17.41, \$24.51, \$25.74 and \$27.03 million respectively.

3.5.1.1 Revenue estimation

1. Direct Revenue

There are two extreme possibilities for direct revenue. One is optimistic, in which biodiesel may have a huge market demand and all biodiesel produced may be sold. The other is pessimistic, in which there is no demand for biodiesel in the market and the biodiesel produced is not sold. The current plant production capacity is 5625 kg/h of biodiesel. From an optimistic view, at a selling price of \$1.173/l, the annual revenue obtained only by the sale of biodiesel is \$62.10 million. From a pessimistic view, there may be no revenue as none is sold. With today's high-energy demand, this possibility is unlikely. The possibility of demand falling between these two extreme possibilities is discussed in the probabilistic risk analysis of revenue estimation.

2. Indirect Revenue

Other than producing 5625 kg biodiesel on an hourly basis, the biodiesel production plant produces 579, 469 and 146 kg of glycerol, FFA and sodium chloride respectively. At their respective selling prices, the annual revenue generated by these products is $6.03, $5.95 and $0.1 million respectively. The sum of the total indirect revenue is $12.08 million. The sum of direct and indirect revenue is $74.18 million (before taxes). The results show that the major contribution to revenue is from the sale of biodiesel (84% of total revenue generated). The percentage contributions of the revenue from FFA and glycerol are the same. The salt, sodium hydroxide, being less in price value has a negligible revenue contribution compared to the other products.

3. Environmental Benefits

Biodiesel fuel not only helps to reduce energy dependency on fossil fuels but its burning also contributes to a clean environment. Burning of biodiesel fuel produces less carbon dioxide (CO_2), a greenhouse gas, than CO_2 produced by burning petroleum-based diesel. Sheehan and co-workers (Sheehan et al. 1998) reported that a net reduction of 78.45% CO_2 could be achieved for biodiesel compared to petroleum-based diesel. The investor in a biodiesel production plant can avail of this environmental advantage as a benefit to his tax returns (Elms & El-Halwagi, 2010). It was assumed that on average diesel ($C_{12}H_{23}$) had 86% carbon content. According to diesel combustion reaction equation, the stoichiometric principles revealed the amount of carbon dioxide produced by burning a unit mass of diesel is as follows:

$C_{12}H_{23}$ (86% C) + $71/4O_2 \rightarrow 12\ CO_2 + 46/4H_2O$

Amount of CO_2 produced = (44/12)*0.86*(1/12) = 0.26 kg CO_2

For biodiesel from Jatropha oil, it was assumed that on average it had 77.6% carbon content. Similarly, the amount of carbon dioxide produced was as follows:

$C_{19}H_{36}O_2$ (77.6% C) + $27O_2 \rightarrow 19CO_2 + 18H_2O$

Amount of CO_2 produced = (44/12)*0.776*(1/19) = 0.15 kg CO_2

For current biodiesel plant capacity, Table 3.5 shows the amount of money that an investor can earn and save, as environmental benefits, by producing biodiesel instead of investing in diesel. The calculations are based on the amount of carbon dioxide released by burning biodiesel and diesel and the dollar value of carbon dioxide emitted.

Table 3.5 CO2 emission

Quantity	Biodiesel fuel	Diesel fuel
Amount of carbon dioxide (CO_2) released by burning of unit amount of fuel (kg/kg)	0.15	0.26
Total biodiesel production capacity (gal)	20203590	
Total CO_2		
Carbon dioxide (CO_2)/biodiesel (tonne/gal)	0.000482	0.000818
Carbon dioxide (CO_2) (tonne)	9749	16542
Dollar value		
US$ per tonne of emitted CO_2	22.22*	
US$	216645	367565
Tax saving (US $million)	0.15	

*(1AUD = 0.94 USD)

The results show that the environmental tax paid for using diesel is higher than for biodiesel. The amount saved is an environmental incentive and is considered as tax-savings for biodiesel investors. The production of biodiesel instead of diesel can save a tax of USD $0.15 million in terms of environmental benefits. It is worth mentioning here that there is still a debate on the applicability and implementation policies of carbon taxes (Smith, 2012). These tax calculations are based on per kg of fuel however; these calculations could also be performed based on per unit energy contents or heating value of the respective fuels. According to the plant start-up schedule, the revenue estimated for year 0, 1, 2, 3, 4, 5 were \$0, \$0, \$41.00, \$90.20, \$99.22 and \$109.14 million.

3.5.1.2 Cost- Benefit analysis

In the current study, the project benefits were calculated using the total revenue (after tax) and total cost of production. The benefit to costs (B/C) ratio analysis was performed with and without environmental benefits. Assuming a sales tax of 13% on revenue collected, the total annual revenue is USD \$64.54 million. At a total cost of USD \$33.38 million, the project's net profit is USD \$31.16 million. This profit does not include environmental benefits. At this stage, the benefit to cost ratio is 0.93. The use of biodiesel instead of petroleum-based diesel reduces the cost value by USD \$0.15 million. Incorporating this environmental benefit as profit, the net benefit is USD \$31.31 million. At the same total cost, the benefit to cost ratio is 0.94. The results show that the project seems less profitable without the addition of environmental benefits, which indicates a high biodiesel production cost and less profit. In order to make a project more profitable, it is recommended to incorporate environmental benefits into the study. The results of benefits-to-cost ratio, presented here, are for total revenue and total cost. The results of benefits-to-cost ratio in the time domain are discussed in the probabilistic cost risk analysis.

3.5.2 Probabilistic Risk Analysis

3.5.2.1 Probabilistic cost risk analysis and cost-benefit analysis- without time domain

The probabilistic cost risk analysis was carried out by assigning triangular distributions to the most likely cost value of individual elements. Triangular distribution was the most appropriate distribution for this study as this was a bounded system where the upper and lower limit and most likely cost were known. Table 3.6 shows the low and high values around the most likely values.

Table 3.6 Uncertainty analyses for cost estimation

Sr. No.	Item	Estimated or most likely cost ($\times 10^{-4}$)	Low or minimum cost ($\times 10^{-4}$)	High or maximum cost ($\times 10^{-4}$)
	Equipment list			
1	R-101	15.47	13.92	17.02
2	S-202	1.44	1.30	1.59
3	S-203	9.28	8.35	10.21
4	S-204	8.25	7.43	9.08
5	S-205	9.80	8.82	10.78
6	S-206	1.03	0.93	1.13
7	S-208	8.77	7.89	9.64
8	ST-202	10.83	9.75	11.91
9	ST-203	4.38	3.95	4.82
10	ST-204	0.99	0.89	1.09
11	ST-206	1.30	1.17	1.43
12	ST-208	3.00	2.70	3.30
13	ST-210	0.44	0.39	0.48
14	M-101	2.50	2.25	2.75

	Fixed capital cost			
15	Equipment erection	30.81	27.73	33.89
16	Piping	53.92	48.53	59.31
17	Instrumentation	15.40	13.86	16.95
18	Electrical	7.70	6.93	8.47
19	Building process	11.55	10.40	12.71
20	Utilities	38.51	34.66	42.36
21	Storage	11.55	10.40	12.71
22	Site development	3.85	3.47	4.24
23	Ancillary building	11.55	10.40	12.71
24	Design and Engineering	78.56	70.71	86.42
25	Contractor's fee	13.09	11.78	14.40
26	Contingency	26.19	23.57	28.81
	Variable cost			
27	Raw material	919.49	827.54	1011.43
28	Miscellaneous materials	3.80	3.42	4.18
29	Utilities	28.35	25.51	31.18
30	Shipping and packaging	150.00	135.00	165.00
	Fixed cost			
31	Maintenance	37.97	34.18	41.77
32	Operating labor	423.83	381.45	466.21
33	Laboratory cost	84.78	76.29	93.24
34	Supervision	84.78	76.29	93.24
35	Plant overhead	211.91	190.72	233.11
36	Capital charges	56.96	51.26	62.66
37	Insurance	3.80	3.42	4.18
38	Local taxes	7.56	6.80	8.31
39	Royalties	3.80	3.42	4.18

The results listed in Table 3.6 are the detailed cost data for each item and the total cost. Highlights of Table 3.6 are shown in Figure 3.5. The Figure 3.5 represents clusters of risk sources which include equipment costs, fixed capital costs, variable costs and fixed costs.

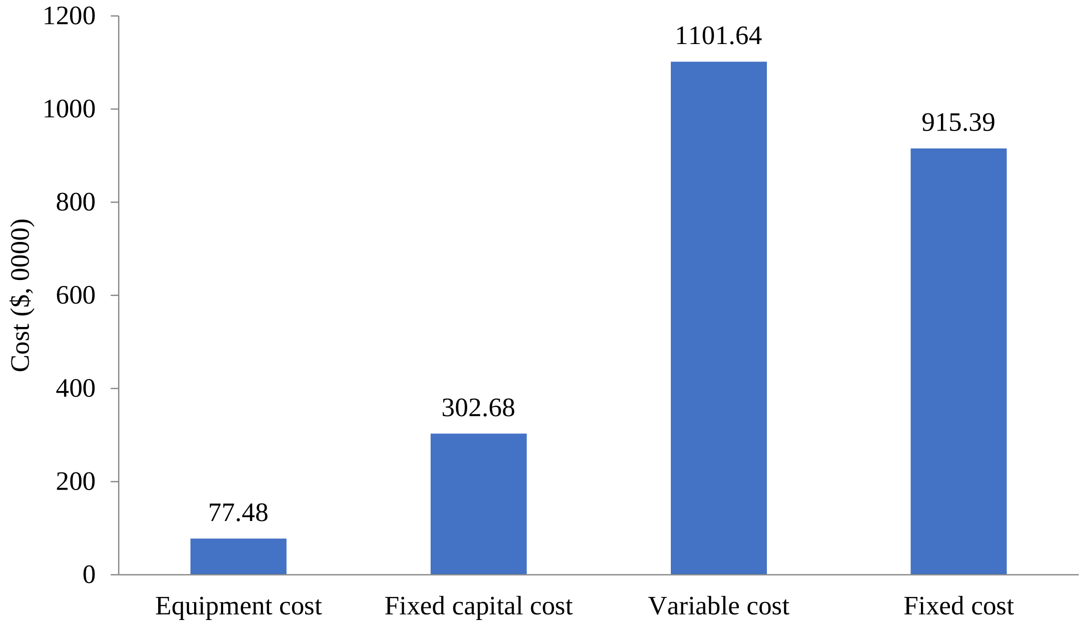


Figure 3.5 Risk sources in cost estimation

Richardson and Mapp (1976) proposed that the probabilities associated with various level of investment are considered as a measure of the risk of the proposed investment. The probabilities associated with the cost exceeding the expected values are identified by the cumulative probability curve, developed for the estimated total cost data. As per plant start-up schedule, for year 0, the cumulative probability curve is developed by performing a Monte Carlo simulation on 30% of the cost value of each item from serial number 1 to 26 in Table 3.6 and the result is illustrated in Figure 3.6.

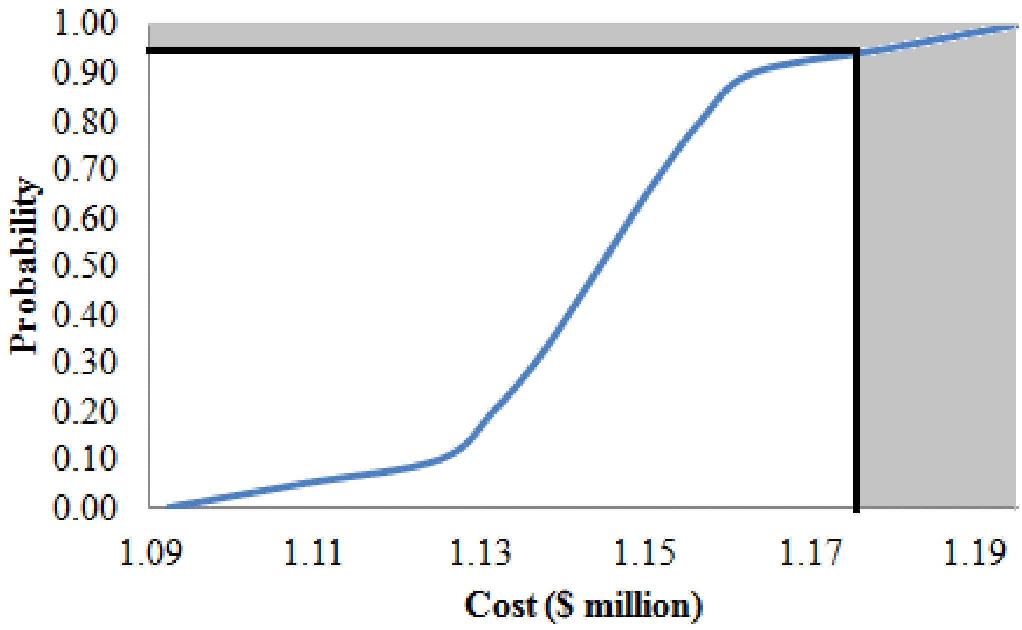


Figure 3.6 Cumulative Probability Distribution of Cost for first year investment

The cumulative probability distribution profile can be analysed at different percentiles. For the current risk analysis, the profile is studied at 5, 20, 60 and 95% values. Figure 3.6 is presented to demonstrate risk estimation at 95% value. In this Figure, at a particular percentile, the cost associated with the target is shown on the horizontal axis. For illustrative purposes 95% value for year 0 and year 1 are discussed in detail.

In Figure 3.6, at 95% value, the cost exceeding the expected value is:

Risk = (1-0.95)*1.174

Risk = $0.0587 million, the grey area in Figure 3.6 represents this risk.

Economic analysis shows the estimated cost for year 0 is $1.96 million; therefore, the actual cost is 1.96 + 0.0587 = $2.018 million. For the next year (year 1), 70% of the estimated cost data from serial numbers 1 to 26 was taken and updated using an inflation rate and interest rate of 5% each. The simulations performed on the cost data of year 1 provided a cumulative distributive plot for the cost of year 1. The cumulative distributive plot was analysed at 5, 20, 40, 60, 80 and 95% values, in the same way as for the first year of investment. At 95% value, the targeted cost was $2.73 million; hence the cost exceeding the expected values for year 1 is:

Risk = (1-0.95)*2.73 = $0.136 million

At the estimated cost of $2.93 million for year 1, the actual cost for year 1 is:

Actual cost = 2.93 + 0.136 = USD $3.066 million

For year 2, since the plant has started its production, there is no fixed capital cost associated. Instead, Monte Carlo Simulation is performed on the variable and fixed cost (from serial numbers 27 to 39) also incorporating the time value of money. Similarly, for the next four years of the project, the results of risk associated with cost of each year at 95% and 40% values are plotted in Figure 3.7, called the cost risk plot. It shows the risk variation over the period of investment. At year 0 and year 1, there is less risk compared to the next years. This is because the plant is being built during this period and there are only capital expenditures associated with the cost; no operational cost is involved. Therefore, the estimated total cost is not very high; hence there is less risk of having this cost value greater than the estimated one. After the plant is operational in year 2 and beyond the risk increases to $1 million, and goes on increasing up to year 5. This shows a huge vagueness in estimated costs. This risk may cause a cost overrun and the plant budget may need additional allocation of funds. The higher the percentile, the lower is the cost risk associated. The cost risk plot is helpful for decision makers to decide how much risk is present in the estimated cost over the period of investment.

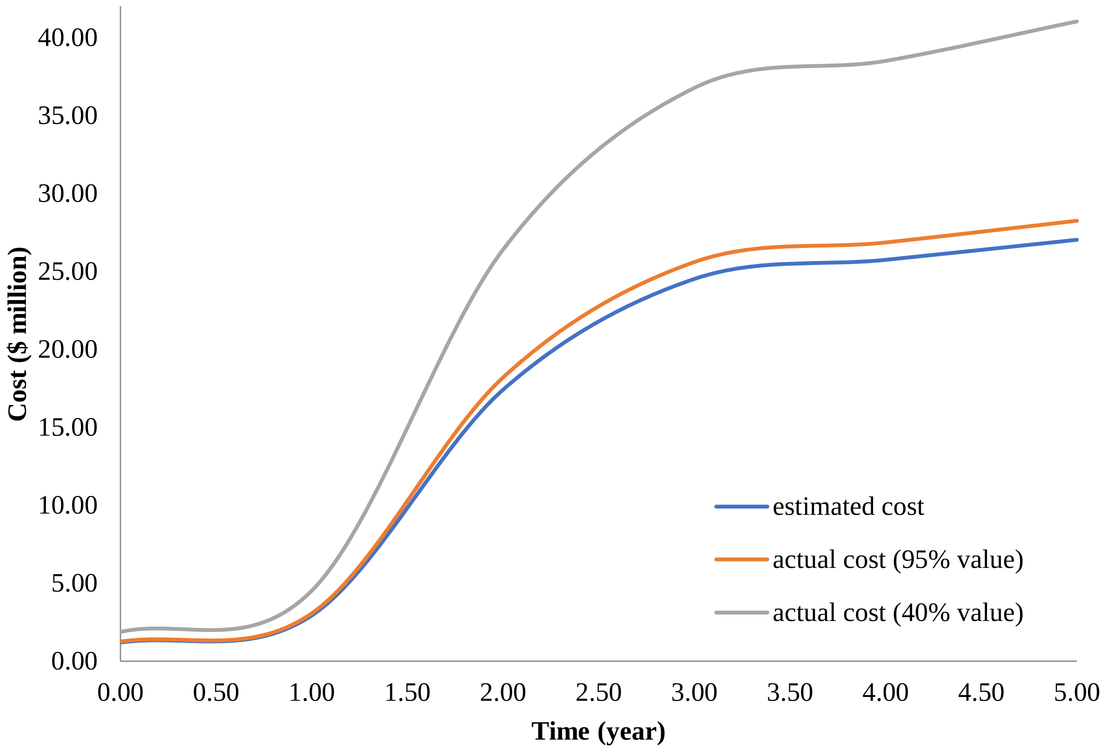


Figure 3.7 Cost Risk Plot: comparison of actual and estimated cost

The estimated cost in Figure 3.7 was evaluated using conventional economic analysis studies discussed in open literature. The actual cost refers to the cost, which includes the probabilistic study of estimated cost data. From Figure 3.7, it is evident that the cost estimated by conventional economic analysis is very vague and does not represent the true picture for economic analysis of process plants, whereas probabilistic risk analysis of estimated cost shows a complete picture. It shows that the actual cost may be far more than the estimated one, depending on the percentile value chosen to represent the cost. Both the actual and estimated cost values were observed to increase with time. Because the cost data at 95-percentile value represent less risk, both curves (estimated cost and actual cost at 95% value) are closer to each other. In the case of actual cost at 40% value, the importance of risk measurement is clearer due to a wide difference between estimated and actual cost. For example, for year 3, the cost estimated by conventional economic analysis of biodiesel plants is \$24.50 million but the probabilistic study shows that the actual cost is \$36.77 million (at 40% value). This represents an increase of \$12.27 million and shows the previously available process economics analyses are lacking in reporting such vagueness. It also shows the importance of current work in order to estimate a risk-free cost. The actual cost based on probabilistic study is more acceptable because both variability of cost data and dynamic cost risk are considered.

Benefit-cost ratio analysis

The results for the probabilistic cost risk analysis disclose that there is a difference between the estimated cost and the cost resulting from risk analysis. This difference can affect the project return period; therefore a benefit to cost ratio analysis was conducted to evaluate the project profitability at the estimated and actual cost. The actual benefits are the benefits (net profits), which include the probabilities of costs exceeding the target values. The benefits, which do not include these probabilities in their costs values, are benefits without including risk. The B/C ratios based on ratios of actual benefits and actual costs for a period of five years are illustrated in Figure 3.8. The risk in cost values was evaluated for 5, 20, 40, 60, 80 and 95 percentiles and the benefits-cost ratio was also evaluated for the corresponding percentiles. To compare the effect of risk on return period, the estimated B/C ratio, involving no risk, is plotted in the same time-domain.

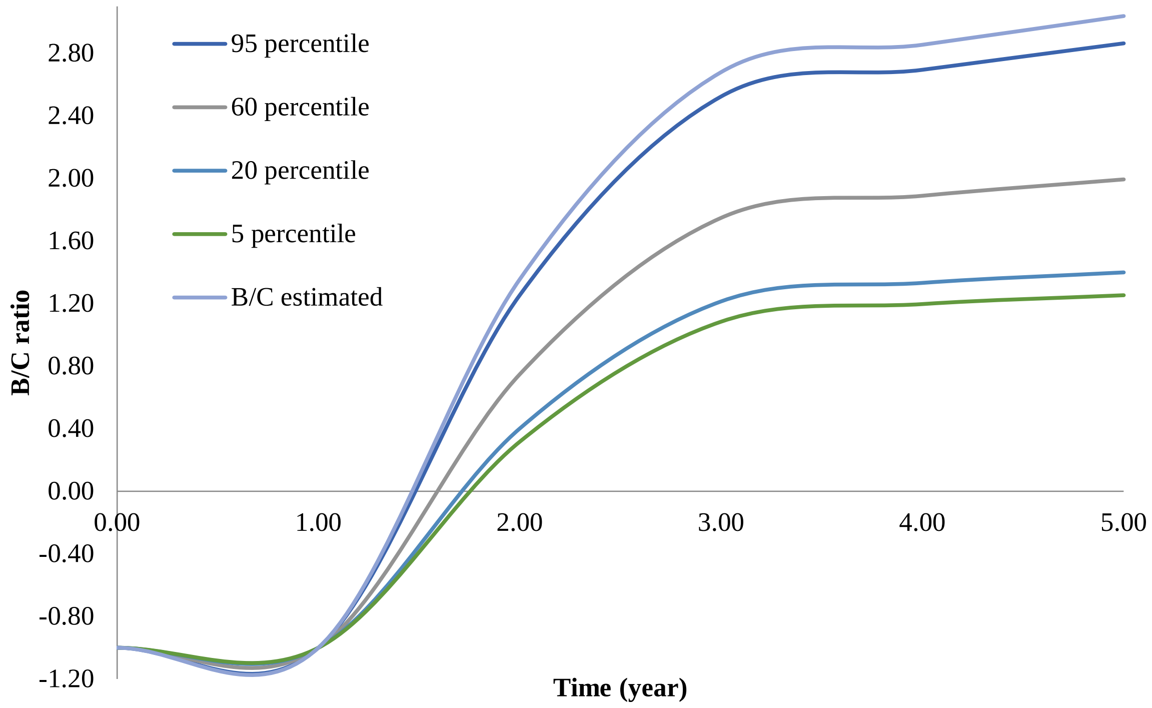


Figure 3.8 Cost benefit analysis for actual and estimated costs

Referring to Figure 3.8, a B/C ratio below zero represents loss and above zero represents that the project is feasible. A B/C ratio of zero shows the revenue earned is equivalent to the cost expenditure and there is no profit earned. The higher the B/C ratio, the higher is the profit earned by the project. The curve of estimated B/C ratio in Figure 3.8 suggests that, in year 2, the project is likely to make a higher profit (B/C = 1.35) after the plant start-up. However, the risk analysis performed shows an entirely different picture. The benefit to cost ratios evaluated at different percentiles show the different levels of risk. The higher the percentile values are, the lower is the risk. At 95% value, the B/C ratio is closer to the estimated B/C ratio since there would be the least risk associated with this value. At 5% value, there is the highest risk and the B/C ratio at this value shows that the project is likely to make much less return (B/C = 0.316). This shows that there is the highest risk of exceeding the cost from the expected value. This is a characteristic of probabilistic economic studies for a biodiesel production plant. The intermediate percentile values show that there are different periods when the project would start making a profit. The analysis shows that according to the previous developed, conventional economic analysis studies for a biodiesel production plant, the plant may start high returns after a few months of investment, but the current study of risk analysis proves its vagueness. It shows that at the highest level of risk, the plant is likely to make much less profit even after 5 years of plant start-up. Referring to Table 3.6, the sensitivity analysis performed on all assumptions shows which assumption has the highest contribution to the variation in total cost data? The results indicate that the major uncertainty in estimating total cost is associated with the cost of raw materials, which contributes 90.7%. This indicates that the cost of raw material has the most influence among all other assumptions and that an adequate source of raw material cost data should be used to lower the risk present in the cost estimation.

3.5.2.2 Probabilistic revenue-risk analysis and cost-benefit analysis

The revenue considered for the current probabilistic study is the revenue (after tax) from direct and indirect categories of revenue. The revenue estimation provides the revenues over the period of production. A Monte Carlo simulation performed on the estimated revenue of year 2 developed the cumulative probability distribution curve and is drawn in Figure 3.9.

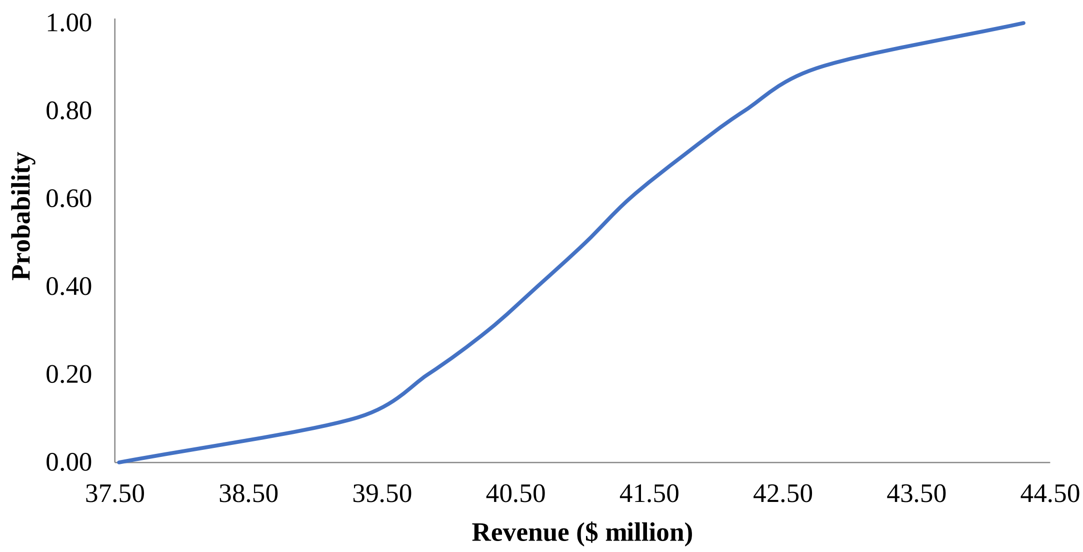


Figure 3.9 Cumulative Probability Distribution of revenue, year 2

The probabilistic distributive curve developed for year 2 is used to evaluate the risk in revenue estimation. The risk for revenue is that the actual revenue may fall behind the expected one. Therefore, the actual revenue is evaluated by subtracting revenue risk from the expected or estimated revenue.

Using Figure 3.9, at 95% value, the revenue below the expected revenue for year 2 is:

Risk = (1-0.95)*43.54 = $2.177 million, hence at the estimated revenue of $41 million for year 2, the actual revenue is:

Actual revenue = 41 – 2.177 = USD $38.823 million

The cumulative plots were developed for years 3, 4 and 5. The cumulative curves were analysed for 5, 20, 40, 60, 80 and 95% values. The results for 95% value are shown in Table 3.7:

Table 3.7 Actual revenue over the period of investment

Year	Risk ($ millions)	Estimated R ($ millions)	Actual R ($ millions)
0	0.000	0.00	0.00
1	0.000	0.00	0.00
2	2.177	41.00	38.82
3	4.754	90.20	85.44
4	5.210	99.22	94.01
5	5.715	109.14	103.43

The relation of revenue risk and time shows that at the start of the production years, there is less risk associated with revenue but in year 5, the risk reaches $5.7 million. This shows the variability in the selling price of biodiesel. There is no risk in year 0 and 1, since the plant is being built during this period and no product is produced or sold so no revenue is earned in this time. The results are helpful for decision makers to analyse how much variability is present in the selling price of biodiesel and how much this might affect the revenue. The plot of revenue estimated from conventional economic analysis versus the actual revenue, the revenue calculated by performing probabilistic economic risk analysis, provides a comparison of both methodologies. The analysis results are shown in Figure 3.10 for actual cost at 95% and 40% values.

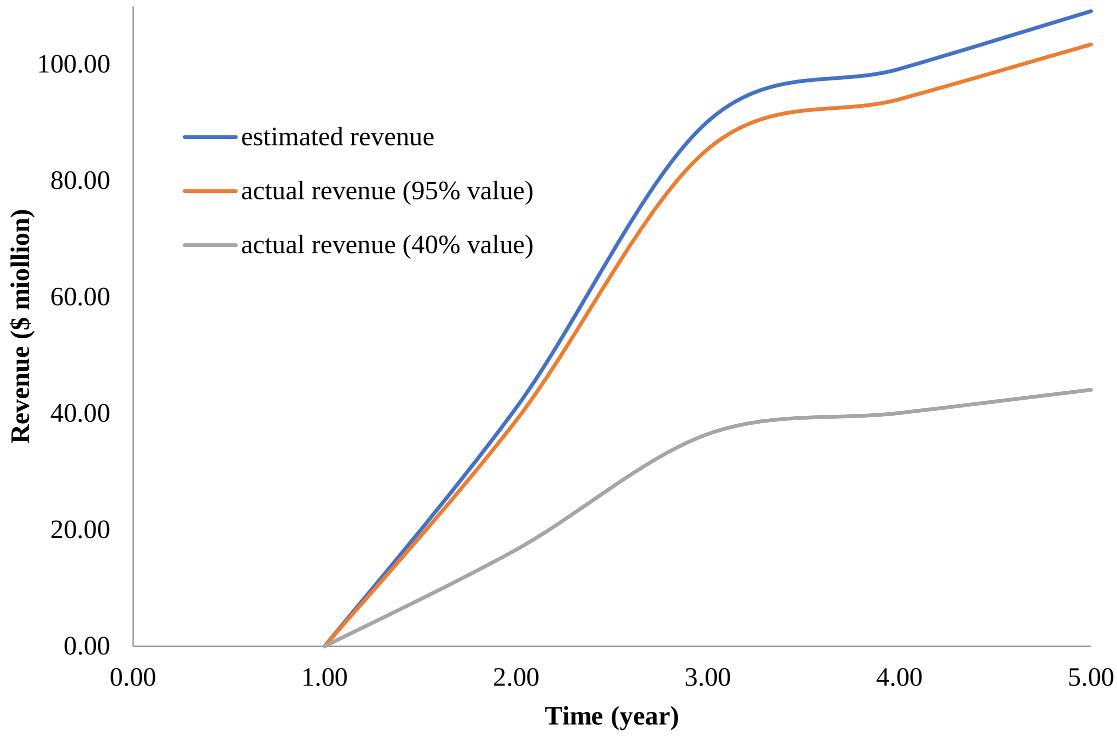


Figure 3.10 Comparison of actual and estimated revenue

Conventional economic analysis results show that the expected and actual revenues would start after year 1 and the amount would increase with time. In the case of revenue estimated by previously available economic analysis, the estimated revenue would be as high as $109.14 million after 5 years of investment. However, in the case of probabilistic risk analysis, the results show a different picture. The probabilistic risk analysis shows that considering a higher risk (40% value); the estimated revenue is much higher than it would be in reality. In the case of 95% value, there is less difference between the actual and estimated revenues since less risk is associated with estimated revenue. The actual revenue figures, involving higher risk, show that the maximum revenue in year 5 would be USD $44 million, which is much less than the revenue of USD $109.14 million estimated by conventional economic analysis studies.

Probabilistic benefit-cost ratio

Since there is a high variation in estimated and actual revenue, the benefit to cost ratio analysis helps to know when the project could be profitable. At the estimated cost values, the actual benefits that include revenue risk and benefits that do not include revenue risk are calculated and the B/C ratio is evaluated. For 5, 20, 40, 60, 80 and 95 percentile values, the graphical results of benefit-to-cost ratio analysis are shown in Figure 3.11.

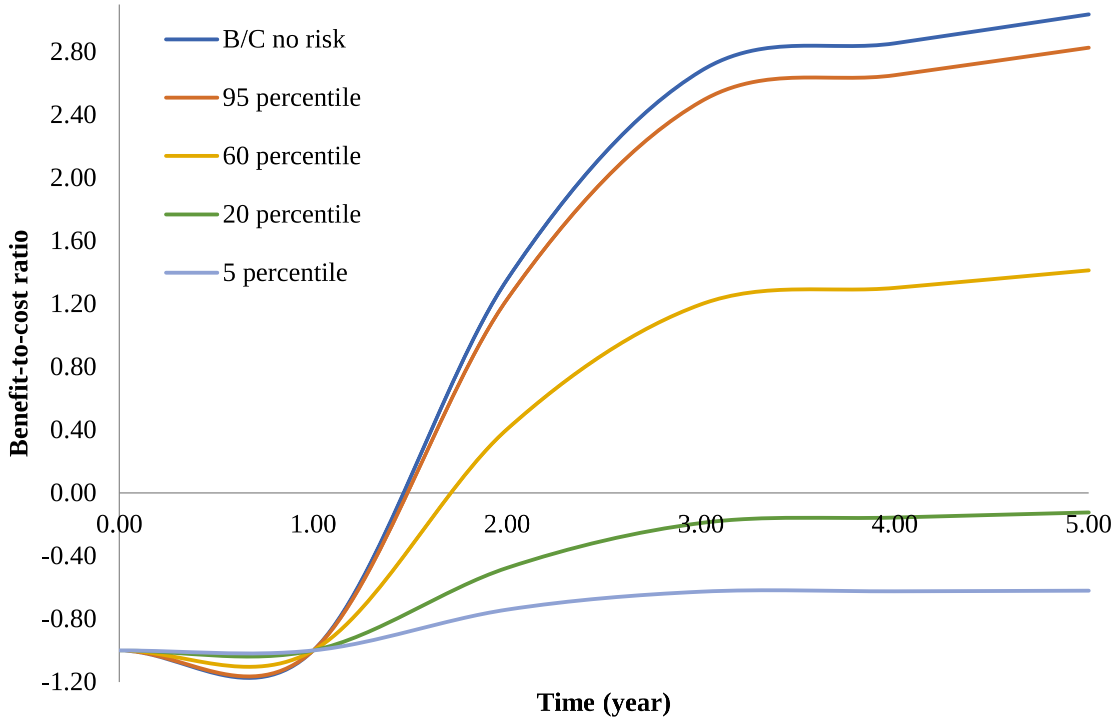


Figure 3.11 Benefit to cost ratio analysis for probabilistic revenue

The economic analysis without the study of risk in estimated revenue (B/C no risk) shows that the project would start its revenue return between year 1 and 2; however, this is not a true picture. When the revenue risk is incorporated, it shows that the project would not start its return even at the end of 5 years of the investment period (20 and 5 percentile values). This indicates that economic risk analysis has more importance than conventional economic analysis since the probabilistic study shows the actual period over which the plant would start its return. Figure 3.11 demonstrates that at higher percentile values there is less risk associated with revenue since the 95% value is much closer to the benefit to cost ratio involving no risk of the estimated revenue, since there is the least risk associated with this percentile. However, as the percentile values are lowered, the risk becomes higher and very significant and at 80% value, the analysis shows that, in year 3, the B/C ratio is 1.92 instead of 2.67 reported as estimated revenue in the same year. This shows the project actually may produce less profit than estimated by the usual economic analysis methods. The least percentile value (5%) shows the highest risk in revenue. This percentile shows that the project is not able to generate profit even after 5 years of the initial investment period. The sensitivity analysis performed on revenue elements indicates that among all products, biodiesel revenue has the highest contribution (82.4%) towards the variation in revenue. Free fatty acid (10.2%) and glycerol (4.1%) have the second and third highest contributions respectively.

3.5.2.3 Probabilistic risk analysis on major equipment of PFD

To produce biodiesel on a large scale, various types of equipment are used. The cost of each piece of equipment varies. As shown in this analysis, the plant's fixed and working capitals are based on total cost of equipment. The vagueness present in the cost of equipment can yield an over- or underestimated cost and may affect the plant's fixed and working capital. As a result, the total production cost estimation may be misleading. Therefore, risk analysis of the cost of each piece of equipment is essential. The results would be helpful in identifying the equipment that needs attention in its cost estimation. The results would also help to know which equipment has the highest cost risk associated with it, because the economic analysis results show the estimated cost of each piece of equipment. The Monte Carlo simulation performed on each piece of equipment developed the cumulative distributive curves of the respective equipment. The cumulative distributive curve of a trans-esterification reactor, the most important equipment in biodiesel production, is shown in Figure 3.12.

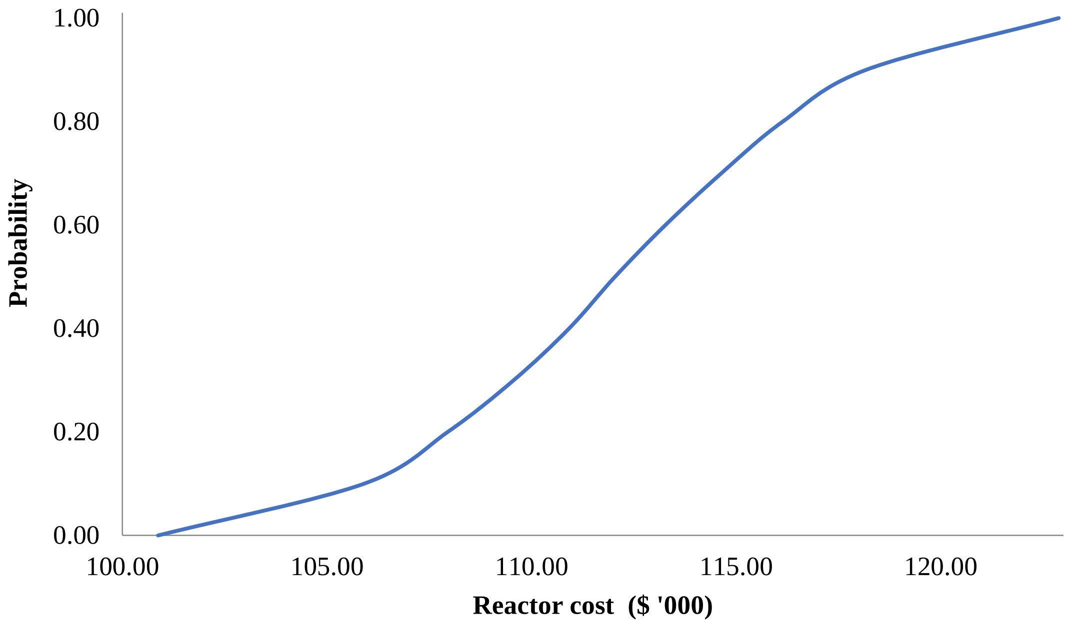


Figure 3.12 Cumulative distributive plot for cost of reactor

At 95% value, the risk of exceeding the reactor cost from the expected cost is:

Risk = (1-0.95)*120,531 = $6,027

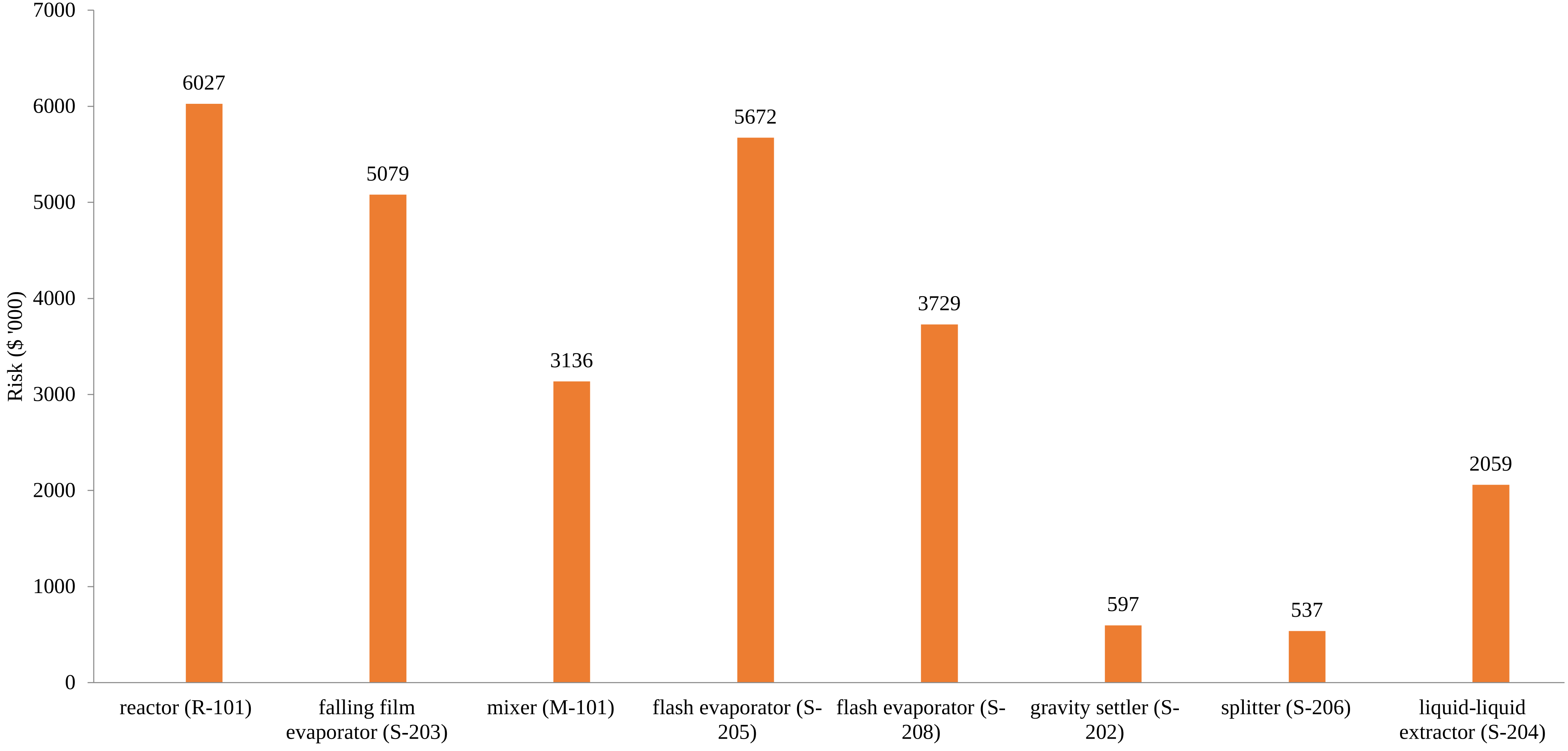


Figure 3.13 Risk associated with different equipment

The risk evaluated for a single piece of equipment using the cumulative plot for different equipment were analysed at 95% value and the results are plotted in Figure 3.13. It shows that the reactor has the highest risk associated with its cost estimation, followed by the flash evaporator (S-205) and then the falling film evaporator (S-203). The least risk is associated with the splitter (S-206). The results provide useful information for decision makers, who should focus on cost estimation of the reactor, flash evaporator and the falling film evaporator more precisely, since the cost of these equipment has the highest risk associated. While performing the economic analysis of a biodiesel production plant, the careful cost estimation of these three pieces of equipment would guarantee that the project would not fail or become uneconomical.

3.6 Conclusions

This research developed an economic risk analysis methodology which was demonstrated on a biodiesel production plant. The raw material for biodiesel production was jatropha oil – inedible oil. The study dealt with uncertainties in estimated cost and revenue data used in biodiesel economic analysis. The probabilistic risk analysis showed the period of the investment when the biodiesel production was economically viable. A probabilistic risk analysis was first performed on the estimated cost data. The analysis revealed that at a lower level of risk, there was less difference between the actual cost and the estimated one. However, at the higher level of risk, the cost estimated by conventional economic analysis was much less than the cost found by the probabilistic study. The vagueness present in the cost data influenced the project return period. To deal with this problem, a probabilistic cost-benefit analysis approach was developed. Results from the probabilistic cost-benefit analysis showed that the project would yield less profit and that the return period is delayed. To address the issue of variability in the selling prices, the second part of the study focused on probabilistic revenue risk analysis and probabilistic risk analysis of major equipment. Results of probabilistic revenue risk analysis showed that the estimated revenue does not represent the actual revenue and the actual revenue is lower than the estimated one due to the variability present in the selling price of biodiesel. The analysis results indicated that the reactor had the highest risk associated with its cost estimation, followed by the flash evaporator. For future work, it is recommended to implement this methodology for other renewable energy systems since cost is also an important factor for such systems.

3.7 References

Abbaszaadeh, A., Ghobadian, B., Omidkhah, M. R., & Najafi, G. (2012). Current biodiesel production technologies: A comparative review. Energy Conversion and Management, 63, 138-148. doi:10.1016/j.enconman.2012.02.027

Balat, M. (2011). Potential alternatives to edible oils for biodiesel production – A review of current work. Energy Conversion and Management, 52(2), 1479-1492. doi:10.1016/j.enconman.2010.10.011

Banković-Ilić, I. B., Stamenković, O. S., & Veljković, V. B. (2012). Biodiesel production from non-edible plant oils. Renewable and Sustainable Energy Reviews, 16(6), 3621-3647. doi:10.1016/j.rser.2012.03.002

Borghi, D. d., Abreu, C. R., & Guirardello, R. (2012). Thermochemical properties estimation for biodiesel related mixtures. Brazil: EngOpt 2012, 3rd International Conference on Engineering Optimization.

CEPCI. (2014). Chemical Engineering's Plant Cost Index (CEPCI). Retrieved February 22, 2014, from www.che.com

Chemical Business, I. (2013). Indicative Chemical Prices A-Z. Retrieved July 10, 2014, from ICIS: http://www.icis.com/chemicals/channel-info-chemicals-a-z/

Ciais, P., Sabine, C., Bala, G., Bopp, L., Brovkin, V., Canadell, J., . . . Thornton, P. (2013). Carbon and other biogeochemical cycles. In T. F. Stocker, D. Qin, G.-K. Plattner, M. M. Tignor, S. K. Allen, J. Boschung, . . . P. M. Midgley (Eds.), Climate Change 2013: The Physical Science Basis. Working Group I Contribution to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change (pp. 465-570). Cambridge, United Kingdom and New York, NY, USA: Cambridge University Press.

Clean Energy, R. (2012). Clean Energy Regulator, Australian Government- Carbon Pricing Mechanism. Retrieved December 12, 2013, from http://www.cleanenergyregulator.gov.au/Carbon-Pricing-Mechanism/About-the-Mechanism/Pages/default.aspx

Cynthia, O.-B., & Teong, L. K. (2011). Feasibility of Jatropha Oil for Biodiesel: Economic Analysis. Linkoping: World Renewable Energy Congress 2011-Sweden.

Elms, R. D., & El-Halwagi, M. M. (2010). The effect of greenhouse gas policy on the design and scheduling of biodiesel plants with multiple feedstocks. Clean Technologies and Environmental Policy, 12(DOI 10.1007/s10098-009-0260-1), 547-560.

Energy, U. D. (2013). Clean Cities Alternative Fuel Price Report - January. U.S Department of Energy, Energy Efficiency & Renewable Energy.

Haas, M. J., McAloon, A. J., Yee, W. C., & Foglia, T. A. (2006). A process model to estimate biodiesel production costs. Bioresource Technology, 97(4), 671-678. doi:10.1016/j.biortech.2005.03.039

Hawash, S., Diwani, G. E., & Kader, E. A. (2011). Optimization of biodiesel production from Jatropha oil by heterogeneous base catalysed transesterification. International Journal of Engineering Science & Technology, 3(6), 5242-5251.

Himmelblau, D. M., & Riggs, J. B. (2012). Basic Principles and Calculations in Chemical Engineering (Prentice Hall International Series in the Physical and Chemical Engineering Sciences) (3rd ed.). (8th, Ed.) United States (US): Prentice Hall.

Kalnes, T., Marker, T., & Shonnard, D. R. (2007). Green diesel: a second generation biofuel. International Journal of Chemical Reactor Engineering, 5th(Article A48), Article A48.

Kasteren, J. v., & Nisworo, A. (2007). A process model to estimate the cost of industrial scale biodiesel production from waste cooking oil by supercritical transesterification. Resources, Conservation and Recycling, 50(4), 442-458. doi:10.1016/j.resconrec.2006.07.005

Keera, S., Sabagh, S. E., & Taman, A. (2011). Transesterification of vegetable oil to biodiesel fuel using alkaline catalyst. Fuel, 90(1), 42-47. doi:10.1016/j.fuel.2010.07.046

Kumar, G. R., Ravi, R., & Chadha, A. (2011). Kinetic studies of base-catalyzed transesterification reactions of non-edible oils to prepare biodiesel: The effect of co-solvent and temperature. Energy and Fuels, 25(7), 2826–2832. doi:10.1021/ef200469u

Kywe, T. T., & Oo, M. M. (2009). Production of biodiesel from Jatropha oil (Jatropha curcas) in pilot plant. Proceedings of World Academy of Science, Engineering & Technology, (pp. 477-483).

Lapuerta, M., Rodriguez-Fernandez, J., & Oliva, F. (2010). Determination of enthalpy of formation of methyl and ethyl esters of fatty acids. Chemistry and Physics of Lipids, 163(2), 172-181. doi:10.1016/j.chemphyslip.2009.11.002

Lopes, D. d., Neto, A. J., Mendes, A. A., & Pereira, D. T. (2013). Economic feasibility of biodiesel production from Macauba in Brazil. Energy Economics, 40, 819-824. doi:10.1016/j.eneco.2013.10.003

Myint, L. L., & El-Halwagi, M. M. (2009). Process analysis and optimization of biodiesel production from soybean oil. Clean Technologies and Environmental Policy, 11(3), 263-276. doi:10.1007/s10098-008-0156-5

Nagarajan, S., Chou, S. K., Cao, S., Wu, C., & Zhou, Z. (2013). An updated comprehensive techno-economic analysis of algae biodiesel. Bioresource Technology, 145, 150-156. doi:10.1016/j.biortech.2012.11.108

Nasir, N., Daud, W., Kamarudin, S., & Yaakob, Z. (2013). Process system engineering in biodiesel production: A review. Renewable and Sustainable Energy Reviews, 22, 631-639. doi:10.1016/j.rser.2013.01.036

Peters, M. S., Timmerhaus, K. D., & West, R. (2002). Plant Design and Economics for Chemical Engineers (5th ed.). McGraw-Hill Book Company.

Rahman, K. M., Mashud, M., Roknuzzaman, M., & Al Galib, A. (2010). Biodiesel from Jatropha oil as an alternative fuel for diesel engine. International Journal of Mechanical & Mechatronics IJMME-IJENS, 10(3), 1-6.

Raja, S. A., Smart, D. R., & Lee, C. L. (2011). Biodiesel production from Jatropha oil and its characterization. Research Journal of Chemical Sciences, 1(1), 81-87.

Richardson, J. W., & Mapp, H. P. (1976). Use of probabilistic cash flows in analyzing investments under conditions of risk and uncertainty. Southern Journal of Agricultural Economics, 8(2), 19-24.

Richardson, J. W., Herbst, B. K., Outlaw, J. L., & Gill II, R. C. (2007). Including risk in economic feasibility analyses: The case of ethanol production in Texas. Journal of Agribusiness, 25(2), 115-132.

Sheehan, J., Camobreco, V., Duffield, J., Graboski, M., & Shapouri, H. (1998). Life cycle inventory of biodiesel and petroleum diesel for use in an urban bus.

Colorado US: National Renewable Energy Laboratory, United States Department of Energy.

Sinnott, R. (2005). Chemical Engineering Design, Coulson and Richardson's Chemical Engineering Series (4th ed., Vol. 6). Oxford, UK: Elsevier Butterworth-Heinemann.

Smith, N. (2012). Carbon taxes won't work. Here's what will. Retrieved December 22, 2013, from http://noahpinionblog.blogspot.ca/2012/06/carbon-taxes-wont-work-heres-what-will.html

Towler, G., & Sinnott, R. (2012b). Excel Templates. Retrieved March 18, 2014, from Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design: http://booksite.elsevier.com/9780080966595/content/Templates/Economic_Analysis.xls

Towler, G., & Sinnott, R. K. (2012a). Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design (2nd ed.). Butterworth-Heinemann.

Ulrich, G. D., & Vasudevan, P. T. (2004). Chemical Engineering Process Design and Economics: A Practical Guide. Process Publishing Company.

West, A. H., Posarac, D., & Ellis, N. (2008). Assessment of four biodiesel production processes using HYSYS.Plant. Bioresource Technology, 99(14), 6587-6601. doi:10.1016/j.biortech.2007.11.046

Yeboah, A., Naanwaab, C., Yeboah, O., Owens, J., & Bynum, J. (2013). Economic feasibility of sustainable high oilseed-based biofuel production: the case for biodiesel in North Carolina. International Food and Agribusiness Management Review, 16(1), 41-66.

You, Y.-D., Shie, J.-L., Chang, C.-Y., Huang, S.-H., Pai, C.-Y., Yu, Y.-H., & Chang, C. H. (2008). Economic cost analysis of biodiesel production: case in Soybean oil. Energy & Fuels, 22(1), 182-189. doi:10.1021/ef700295c

Yusuf, N., & Kamarudin, S. (2013). Techno-economic analysis of biodiesel production from Jatropha curcas via a supercritical methanol process. Energy Conversion and Management, 75, 710-717. doi:10.1016/j.enconman.2013.08.017

Zhang, Y., Dube, M., McLean, D., & Kates, M. (2003a). Biodiesel production from waste cooking oil 1. Process design and technological assessment. Bioresource Technology, 89(1), 1-16. doi:10.1016/S0960-8524(03)00040-3

Zhang, Y., Dube, M., McLean, D., & Kates, M. (2003b). Biodiesel production from waste cooking oil: 2. Economic assessment and sensitivity analysis. Bioresource Technology, 90(3), 229-240. doi:10.1016/S0960-8524(03)00150-0

Chapter 4

4 Integration of interpretive structural modelling with Bayesian network for biodiesel performance analysis

Authorship and contributorship

This work has been published by Sajid, Z., Khan, F., & Zhang, Y. (2017). "Integration of interpretive structural modelling with Bayesian network for biodiesel performance analysis". *Renewable Energy*, 107, 194-203".

An online as well as a pdf file of this paper can be accessed through following link: http://www.sciencedirect.com/science/article/pii/S096014811730068X

The co-author, Dr. Faisal Khan, formulated the research problem. The first author, Zaman Sajid, structured the approach, designed and conducted the analysis, executed the assessment and drafted the manuscript. The co-authors, Drs. Faisal Khan & Yan Zhang, critically reviewed the developed approach, improved both the approach and manuscript by providing further suggestions. Zaman Sajid incorporated feedback from co-authors and also from the peer reviewers for publication.

Abstract

The performance of a biodiesel system can be affected by varied risk factors. The numbers of such risk factors are large and their interdependencies are vague and complex. The purpose of this study is to define relationships among such risk factors and integrate them with an objective risk analysis approach. In the present study, an interpretive structural modelling (ISM) approach was used to identify relationships among risk factors while a Bayesian Network (BN) approach was employed to define the strength of dependence and conduct a risk analysis. The results indicate that among 25 risk factors, operational safety is a key biodiesel performance factor. The analysis also highlights that the impacts of occupational health and natural resources depletion are strongly dependent on environmental parameters. Occupational health is also strongly dependent on plant safety. The results show that the interdependency between occupational health and natural resources depletion is weak.

4.1 Introduction

With population growth, the demand for energy, and particularly fossil fuels, is on the rise. This growing demand to consume fossil fuels has led scientists to explore innovative technologies to produce alternate energy resources. Of potential alternative energy sources, biodiesel seems to be a promising one. Biodiesel, which is produced by a trans-esterification reaction, has been produced using various new methods and alternate raw materials (Achten, Verchot et al. 2008, Demirbas and Demirbas 2010, Srinivas and Satyarthi 2010, Atabani, Silitonga et al. 2013, Fu, Song et al. 2015, Azeem, Hanif et al. 2016, Guldhe, Singh et al. 2016). Technological innovations in biodiesel production processes have also introduced various uncertainties. In terms of performance, there are various risk categories, which could be characterized to study biodiesel performance risk factors. The nature of the interdependencies of such risk factors has not been studied to date. A well-developed biodiesel performance risk management system requires the identification of biodiesel performance factors as the first step. However, identification of such factors and their quantitative dependency is quite vague and no research has been done in this area.

This paper aims to analyse the risk factors affecting biodiesel production and their use, henceforth referred to as a biodiesel performance system. The interdependencies of biodiesel production and use were studied by implementing interpretive structural modelling (ISM). A Bayesian Network (BN) approach was integrated with ISM to identify the strength of such interdependencies and to conduct a risk analysis. A brief review of the applications of ISM in engineering analysis is presented below.

Warfield (1974) proposed interpretive structural modelling (ISM) which was used to develop a visual hierarchical structure of complex systems. The technique was used in managing decision-making for complex problems. The input for the ISM technique was unstructured and used unclear information about the system variables and their interdependencies. The output of ISM analysis was a well-defined, classified and informative model, which is useful for many other purposes.

Pfohl et al. (2011) implemented ISM to study the interdependencies in supply chain risks. The interrelationship among supply risk factors, they developed, was based on the dependence and driving power of respective factors. Their study was helpful to supply chain risk managers making decisions about resources management. They studied 21 risk factors and initial interrelationships were developed using group discussions among the authors and fellow researchers.

Singh et al. (2008) structured nine barriers in knowledge management (KM) in business strategy. The KM barriers were those, which adversely affect the implementation of KM in a business organization. They implemented ISM methodology for their studies. The mutual relationships among different barriers were classified in different levels and included a visual correlation as well. However, the study was lacking in explaining how weak or strong relations were among various interconnected factors.

Wang et al. (Wang, Li et al. 2014) have utilized this methodology to determine the correlations of risk factors in an Energy Performance Contracting (EPC) project. The applications of ISM to their EPC project resulted in a five-level hierarchical model using EPC project risk factors. There were 25 risk factors that were studied to develop a visual correlation, categorised in five levels. The study helped stakeholders to manage surface, middle and deep risk factors that affect an EPC project.

ISM has found its applications in various other fields of studies including financial decision making, complex engineering problems, total productive maintenance (TPM), competitive analysis and electronic commerce (Mandal and Deshmukh 1994, Chidambaranathan, Muralidharan et al. 2008, Attri, Grover et al. 2012, Govindan, Azevedo et al. 2015). However, implementation of ISM for a process system has been less studied. As is evident, most previous studies have implemented ISM to study the qualitative relationships among different factors. However, only a few of those studies have developed a quantitative relation among those factors. Since the development of a qualitative relationship does not predict whether the relationship is weak or strong, there is a need to develop a model, which shows such strength relations. Until today, biodiesel production systems have been much studied from their economic and environmental aspects. For example, there have been various studies on biodiesel process economics (Haas, McAloon et al. 2006, van Kasteren and Nisworo 2007, Apostolakou, Kookos et al. 2009, Sajid, Zhang et al. 2016) and the related environmental impacts (Kim and Dale 2005, Lardon, Hélias et al. 2009, Marulanda 2012, Sajid, Khan et al. 2016). These studies have considered the economic and environmental aspects of a biodiesel production system using new and different raw materials and production technologies. However, these studies have not considered the performance of the biodiesel production system. Since the production of biodiesel is affected by various performance risk factors, considering only economic and environmental impacts made such studies vague and do not represent a complete picture of a biodiesel production system. Moreover, previous studies do not consider ways to better maintain the performance of a biodiesel system.

As mentioned earlier, this study integrates ISM and BN to conduct a biodiesel system performance risk analysis. The study considers biodiesel performance in three dimensions: i) process, ii) design and installation and iii) operations. This study is helpful to analyse biodiesel performance throughout the process life cycle. It assists in identifying bottlenecks throughout the life cycle of biodiesel and factors affecting these bottlenecks. Swift actions can be taken to overcome bottlenecks to bring biodiesel closer to being a green, safe and economic alternative fuel.

4.2 Problem definition

A biodiesel life cycle and economics study relies on various biodiesel performance risk factors. These risk factors are widespread in various performance dimensions and only a vague picture of their hierarchical order is present, which indicates that the impact of one risk factor on others or over a whole network is quite ambiguous. Therefore, there is a need to develop a qualitative as well as quantitative relationship among such risk factors. The qualitative relationship provides the interdependencies among various risk factors and quantitative analysis provides the strength among those risk factors. In order to perform such an analysis, three dimensions of biodiesel performance are included in this study, namely process, design and installation and operations. This study does not include technological modifications in vehicles or infrastructure for the use of biodiesel as fuel or the performance of biodiesel blends with diesel fuels. The stages of process performance under the study are technological maturity, size and complexity, organizational support, costs, benefits, environmental impacts, safety and risk management. In terms of design and installation, the various stages under study are regulatory, technical and financial compliance. Also under study are suppliers, intellectual property rights and organizational and strategic components. The stages of operational performance include environmental, health and safety risks, flexibility, engineering features, reliability, operational effectiveness, technological innovation and profitability. The input data for this study were the development of the binary contextual relationships among risk factors, using experts' opinions. The experts were a research group of a senior University professor, who has an extensive knowledge and a broad experience in process engineering research and development. Various risk factors for process, design and installation and operations categories are shown in Table 4.1, Table 4.2 and Table 4.3 respectively.

The main objective of this article is to investigate interdependency of various biodiesel performance risk factors and to study the quantitative strength of their relationships using conditional and marginal probabilities. Due to space limitations, the application of the methodology developed for all risk factors is not possible. Hence, a case study of environmental, health and safety risk for operations is chosen to demonstrate methodology. The risk category of environmental, health and safety risk consisted of five risk factors: environmental concerns, human health, occupational health, plant safety and natural resources.

Table 4.1 Risk factors for process category

Risk Category	Risk factor
Technological maturity	• Process maturity • Process sophistication • Chemical and physical aspects of biodiesel production process
Size and complexity	• Project size • Project complexity • Dependence on other projects • Dependence on individuals • Dependence on suppliers
Organizational support	• Business area involvement • Support from areas affected by the change • Sponsor location • Sponsors • Resource source commitment • Computational operations support • Top management involvement
Costs	• Cost overrun • Cost underestimation • Budget conformity • Financial exposition • Cost estimation accuracy • Contingencies
Benefits	• Benefits reliability • Benefit achievement plan • Benefit measurement • Product demand fluctuation
Environmental Impacts	• Process environmental impact • GHG emissions from plant
Safety	• Process safety • Instrumentation and process control • Personal safety • Equipment safety • Natural disaster damage
Risk management	• Guidelines planning • Quality assurance • Decision-making

Table 4.2 Risk factors for design and installation category

Risk Category	**Risk factor**
Regulatory compliance	• Test compliances • Policy changes • Safety issues • Compliance with new standards • Legal issues with competitors
Technical	• Technical risks - components • Design robustness • Technical aspects of biodiesel production plant design • Technology development meets timeline • Production of technical manuals - tends to be late
Financial	• Relatively high costs for low-quantity components • Correct pricing • Building adequate sales • High initial costs for relatively low sales • Loans - high gearing
Supplier	• Key suppliers - will they deliver? • Supplier changing component specifications • Reliance on limited number of suppliers
Intellectual property rights	• Developing and protecting IPR • Developing strong branding • Research needed to validate product
Organisational	• Retention of key personnel • Internal competencies • Internal organisational change • Redundancies • Impact on staff through change of location
Strategic	• Timescale for components • Lead time for tooling, bedding-in components • Meeting ideal product launch time frame • Late decision changes • Clarifying/agreeing on objectives • Decision changes by key partners • Overstretched management • Coordinating new product design with external funding deadlines

Table 4.3 Risk factors for operations category

Risk Category	Risk factor
Environmental, health and safety risks	• Environmental concerns • Human health • Occupational health • Plant safety • Natural resources
Flexibility	• Operational robustness • Equipment robustness
Engineering features	• Organizational system • External events
Reliability	• Poor construction • Production lost • Service difficulty • Life risk evaluation • Maintainability
Operational effectiveness	• Operational efficiency • Operational complexity • Operational performance • Supply chain risks of biomass feedstock
Technological innovation	• Technology not defined • Technological testing • Cost efficient technology
Profitability	• Favourable input prices • Favourable output prices • Price volatility

4.3 The Analysis Methodology

This research was performed using a nine-step approach. The work integrated ISM and BN approaches. ISM is an interpretive method which takes into account structural mapping of various risk factors (Pfohl, Gallus et al. 2011). In order to develop the mapping, the risk factors were first defined and then their order of complexity was studied. This provides the influence between the elements. The modelling converts a complex undefined (or badly defined) system into a well-presented and well-organised system, which consists of a directed graph called a digraph. The complex system developed as the digraph is known as a 'basic structural model', the expansion of which leads to an 'interpretive structural model'. The methodology takes into account a group discussion from experts on how the elements are related to each other. The analysis was further enhanced by developing a Bayesian network (BN) model. The BN model helps to quantify the strength of relationships rather than merely considering the qualitative relationships. The definition of strength used here refers to the strength of risk element *i*'s impact on the risk element *j*'s probability of occurrence. Since risk element *i* may or may not occur, the probability concept used is the conditional probability. The schematic flow of the methodology is shown in Figure 4.1. The various steps in ISM modelling are as below.

Step 1: Risk factors identification

In this step, different risk factors were identified related to three categories of biodiesel performance study. Those three categories were 1) process 2) design and installation 3) operations. These categories were sub-categorised using the research/work from previous studies (Zhi 1995, Czuchry and Yasin 2003, Cameron and Raman 2005, Jallow, Majeed et al. 2007, Williams, Inman et al. 2009, Salzano, Di Serio et al. 2010, Christopher, Mena et al. 2011, Nair 2011).

Step 2: Development of contextual relation among variables

In this step, a contextual relationship was developed among the variables identified in step 1. This relationship could be neutral, influential or comparative in nature. A pair-wise relation was studied. If a relation existed between two variables, it was written as Y. If there was no relation, it was written as N. Experts' knowledge was the input for this step.

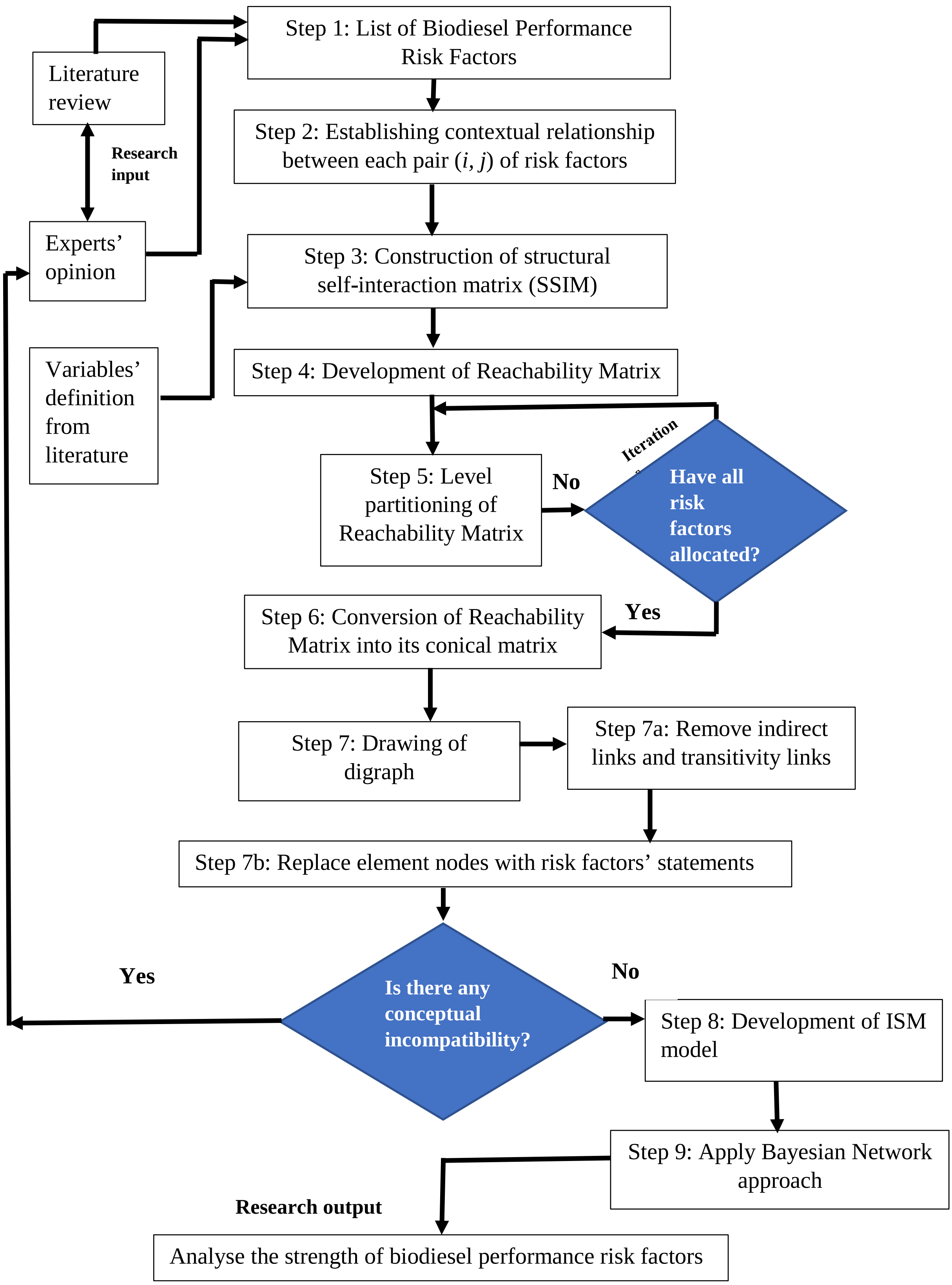


Figure 4.1 The flow diagram of the Analysis Methodology used in the present study

Step 3: Development of structural self-interaction matrix (SSIM)

This step of ISM includes the development of a structural self-interaction matrix (SSIM) through pair-wise comparison of variables correlated in step 2. The contextual relationship developed in step 2 was the input for this step, and the existence between two sub-elements (*i* and *j*) along with their associated direction were questioned. This work is considering binary matrix (*i* x *j*) only, however, the contextual relationship can also be defined for a tertiary matrix (*i* x *j x k*). In the latter case, the contextual relationship should be defined by considering the relation of one element with the pair of elements.

Depending on the variable relation and direction, four different symbols were allocated between the elements *i* and *j*. These variables are as below:

V – When *i* is linked to *j* but *j* does not link to *i*

A – When *j* is linked to *i* but *i* does not link to *j*

X – When *j* is linked to *i* and *i* is linked to *j* (both directions)

O – When the relation between *i* and *j* does not appear to be valid in either direction.

Step 4: Development of reachability matrix (RM) from SSIM

The SSIM developed in step 3 was converted into a reachability matrix (RM) and transitivity was checked in this matrix. RM was a binary matrix in which symbols in step 3 (V, A, X and O) were converted into 0 and 1 using the following rules:

If the pair (*i*, *j*) in SSIM is V, then (*i*, *j*) entry in RM becomes 1 and the (*j*, *i*) entry becomes 0

If the pair (*i*, *j*) in SSIM is A, then (*i*, *j*) entry in RM becomes 0 and the (*j*, *i*) entry becomes 1

If the pair (*i*, *j*) in SSIM is X, then (*i*, *j*) entry in RM becomes 1 and the (*j*, *i*) entry becomes 1

If the pair (*i*, *j*) in SSIM is O, then (*i*, *j*) entry in RM becomes 0 and the (*j*, *i*) entry becomes 0

Using these rules an initial RM was prepared. One of the basic assumptions in ISM is transitivity. This states that if a variable A is related to variable B and if variable B is related to another variable, C, then variable A is also related to variable C. In terms of entries *i* and *j*, if (*i*, *j*) of an RM is 0, there is no direct or indirect relationship from *i* to *j*. Any entry 1* is made to incorporate such transitivity during development of the final RM.

Step 5: Partition of RM into different levels

In this step, reachability R(si) and antecedent A(si) sets were developed using a final reachability matrix. The R(si) consisted of element *i* itself and other elements which it may affect (elements in the row), whereas the A(si) consisted of element *i* and the elements that may affect it (elements in the column). Consequently, the intersection of R(si) and A(si) i.e., R(si) ∩ A(si) was determined. This included the common elements in both R(si) and A(si). A comparison of columns R(si) and R(si) ∩ A(si) was made. The element for which R(si) and R(si) ∩ A(si) are equal, was the top-level element in the hierarchy and the element was assigned level I. The level I elements were the elements which would be at the top of the hierarchy and would not lead other elements above their own level. Once top-level element(s) were identified, they were separated from the pool of the remaining elements. Then the same process was repeated until the level for each element was allocated. These iterations ended when all elements had been allocated their levels. This is worth mentioning here that more than one element can take same level at the same time.

The levels identified are important in developing a digraph and the final ISM model.

Step 6: Development of conical matrix

In this step, elements were arranged in column and row according to their levels, defined in step 5, (level I element, level II element, level III element, level IV element and level V element). This re-arrangement developed a matrix called conical matrix. In this way, all the elements with the same level were pooled together which resulted in most zero (0) elements being in the upper half-diagonal of the matrix and most unitary (1) elements being in the lower half-diagonal of the same matrix.

Step 7: Drawing of a directed graph

Based on the relationship developed in the conical matrix from step 6, a directed graph called a digraph was drawn. In this step, the transitivity links were removed. The elements were arranged according to their level as identified in step 5 and were connected to each other by arrows using the following rules. If an element is connected to another element in the conical matrix (having entry 1), an arrow pointing from this element towards other elements was drawn. If an element was not connected to another one in the conical matrix (having entry 0), no arrow was drawn. The procedure was repeated until the last element in the conical matrix had been connected. The final result (digraph) represented a visual connectivity of all elements and their interconnectivity.

Step 8: ISM model

The resultant digraph from step 7 was converted into an ISM by replacing elements' nodes with their respective statements, the final ISM model was reviewed for any conceptual inconsistency or incompatibilities and modifications were made, if necessary.

Step 9: Bayesian network (BN) Model

A BN is a graphical model that represents random variables using a probabilistic approach. A directed acyclic graph (DAG) developed in step 8 was used to perform this analysis. The DAG consisted of nodes, which represented risk variables or factors and edges represented the causal dependency among various risk factors. This causal dependency was a probabilistic one and was expressed by the structure of the nodes. In a BN, this process provided qualitative causal reasoning. Integrating BN into ISM provided a quantitative model to study the strength of relationships between elements. Previously researchers had used a BN approach in various fields to analyse and manage risks (Pai, Kallepalli et al. 2003; Trucco, Cagno et al. 2008; Lockamy and McCormack 2012; Weber, Medina-Oliva et al. 2012). Based on the conditional dependencies, a BN factorizes the joint distribution of variables. The BN computes the distribution probabilities in a given set of variables by using prior information of other variables (Jensen 1996). The set of nodes and directed arcs are the characteristics of a BN, where nodes represent the system variables and the arc represents the cause-effect relationship or dependencies among the variables. The arcs among the risk factors for biodiesel system performance analysis are drawn using an ISM approach. Each node has its probability of occurrence. In the case of a root node, such probability is an a priori one and is determined for the others by inference. The nodes which are not directed towards any other nodes are the parent nodes. A child node is a node in which a node receives any edge/directed arcs. Probabilities of parent nodes and a conditional probability table (CPT) were the bases for BN computations. The CPT contained the information for conditional probabilities. For instance, for elements A and B, the conditional probability of A, given that B occurs, is written as P(A/B). In this case, B is directed towards A (Weber, Medina-Oliva et al. 2012). In the present study, CPTs were developed by experts' group discussions. Their expertise and their professions have been elaborated earlier in this paper. Bayes' theorem, a theorem proposed by Thomas Bayes, is the basis for the Bayesian network. Bayes' theorem states (Pai, Kallepalli et al. 2003) that

$$P(H/E) = \frac{P(E/H).P(H)}{\sum_{k=1}^{n} P(E/H_k).P(H_k)}$$

where

$P(H/E) =$ Probability of H (being true) given that E occurs

$P(E/H) =$ Probability of E (being true) given that H occurs

P(H) = Prior probability of H occurrence (subjective belief)

$\sum_{k=1}^{n} P(E/H_k).P(H_k) =$ Sum of products of probability of E given every H and probability of H (given that all H are mutually exclusive and exhaustive). A variable elimination (VE) method was used to study the strength among different risk factors. The approach followed a BN study. The methodology included two steps:

1) Defining initial factors and choosing the elimination order
2) Development of factors and algorithm

1) Defining initial factors and choosing the elimination order

For the current case study, the interest was to investigate the positive impact of occupational health on natural resources. The variables were allocated to be used in developing an algorithm. The associated variables in this study were natural resources (N), human health (H), environmental concerns (E), plant safety (P) and occupational Health (T). Based on the defined variables, the objective of the study was to find the probability of occurrence of natural resources given the fact that occupational health would occur i.e., P (N/+T). A positive symbol + symbolizes when an event is sure to occur. Initial factors were P (P), P (N/H, E, P), P (H/E, +T), P (E/P), P (+T/P) and the elimination order was P, E, H.

2) Development of factors and algorithm

New factors were developed by eliminating variables according to the elimination order. These new factors were based on marginal as well as conditional probabilities of initial factors from the digraph. For each elimination variable under study, a new factor was developed by eliminating that variable and the process was repeated until the required objective was attained as shown below.

For Plant Safety P, the factor f1 was:

$$f1\ (N, H, E, +T) = \sum_{\text{(for all possible values of P)}} P\ (P).\ P\ (N/H, E, P).\ P\ (E/P).\ P\ (+T/P)$$

For Environmental Concerns E, the factor f2 was:

$$f2\ (N, H, +T) = \sum_{\text{(for all possible values of E)}} f1\ (N, H, E, +T).\ P\ (H/E, +T)$$

For Human Health H, the factor f3 was:

$f3\ (N, +T) = \sum_{(\text{for all possible values of } H)} f2\ (N, H, +T)$

The probability P (N, +T) is directly proportional to f3:

$P\ (N, +T) = f3\ (N, +T)$

Once the CPT had been established for each risk variable, the algorithm was developed to study the strength among various risk factors in a network, followed by normalization. This means probability values of the final objective are non-zero and the combined value of each CPT is 1. The probability P (N, +T) was renormalized as below:

$P\ (N/+T) = P\ (N, T)/\ P\ (+T)$

4.4 Results and Discussion

For the environmental health and safety category, there were five risk factors identified, namely environmental concerns, human health, occupational health, plant safety and natural resources. The contextual relationships developed by experts show how one risk factor affects another risk factor. The results of the contextual relationship study indicate that the environmental concerns risk factor has a positive effect on human health and natural resources and does not have a negative effect on plant safety and occupational health. Moreover, plant safety has a positive influence on all risk factors under study since plant safety has a core impact on an operational environment. Similarly, keeping in mind the contextual relationship for each individual risk factor and its associated direction, the pairwise relationship developed by experts is shown in Table 4.4.

Table 4.4 Contextual relationships among risk factors

Risk Category: Environmental health and safety risks					
Risk factors	Environmental concerns	Human health	Occupational health	Plant safety	Natural resources
Environmental concerns		Y	N	N	Y
Human health	N		N	N	Y
Occupational health	Y	Y		N	N
Plant safety	Y	Y	Y		Y
Natural resources	N	N	N	N	

Since environmental concerns have a positive effect on natural resources but vice versa is not true, a variable V was assigned for a relationship between both of these variables. Human health has no influence on plant safety; however, vice versa is true; therefore, a variable A was assigned to define the relationship between two variables in an SSIM. An SSIM for the contextual relationships listed above is shown in Table 4.5.

Table 4.5 Structural self-interaction matrix

		5	4	3	2	1
1	Environmental concerns	V	A	A	V	
2	Human health	V	A	A		
3	Occupational health	O	A			
4	Plant safety	V				
5	Natural resources					

The SSIM developed was converted to an RM using the rules mentioned in step 4 of the ISM methodology. The final RM has two characteristics associated with it. First, it provided information about the correlations of risk elements, and secondly, it shows dependence and the driving power of each risk. Driving power is the total number of risks which a risk element affects. This total also includes that risk element. The dependence power of each risk is the total number of risks that affect it, including itself. In other words, the driving power is the sum of interactions in a row and dependence power is the sum of interactions in a column. Table 4.6 represents the RM of the case study under discussion.

Table 4.6 Reachability matrix (RM)

Elements	1	2	3	4	5	Driving Power
1	1	1	0	0	1	3
2	0	1	0	0	1	2
3	1	1	1	0	0	3
4	1	1	1	1	1	5
5	0	0	0	0	1	1
Dependence Power	3	4	2	1	4	

The RM facilitated the levels of risk in a biodiesel performance system. The output of the RM helped to develop reachability set R(si) and antecedent A(si) set which subsequently helped to define the levels for each element in the RM. Top level elements did not have any other elements above them. The process was completed in four iterations starting from element 4 and ending with element 2. The results are represented in Table 4.7.

Table 4.7 Levels of Biodiesel performance risks

Elements	Reachability set R(si)	Antecedent set A(si)	R(si) ∩ A(si)	Level
1	1,2,5	1,3,4	1	III
2	2,5	1,2,3,4	2	II
3	1,2,3	3,4	3	IV
4	1,2,3,4,5	4	4	V
5	5	1,2,4,5	5	I

An analysis of Table 4.7 provides the hierarchical arrangement of elements. The hierarchical arrangement of elements is 5, 2, 1, 3 and 4 and their respective levels are level I for element 5, level II for element 2, level III for element 1, level IV for element 3 and level V for element 4.

Figure 4.2 shows risk factors and their levels in a conical matrix. Based on the relationships in the conical matrix, the initial digraph was developed and after removing indirect links and checking for incompatibilities, the final digraph is obtained.

Figure 4.2 also shows dependency of occupational health on environmental concerns; however, this direct dependency was ignored in ISM (Figure 4.3) since occupational health is indirectly influencing environmental concerns through human health, natural recourses and plant safety respectively. In the final step, the elements' descriptions are written in digraph and this digraph is called an ISM (Figure 4.3).

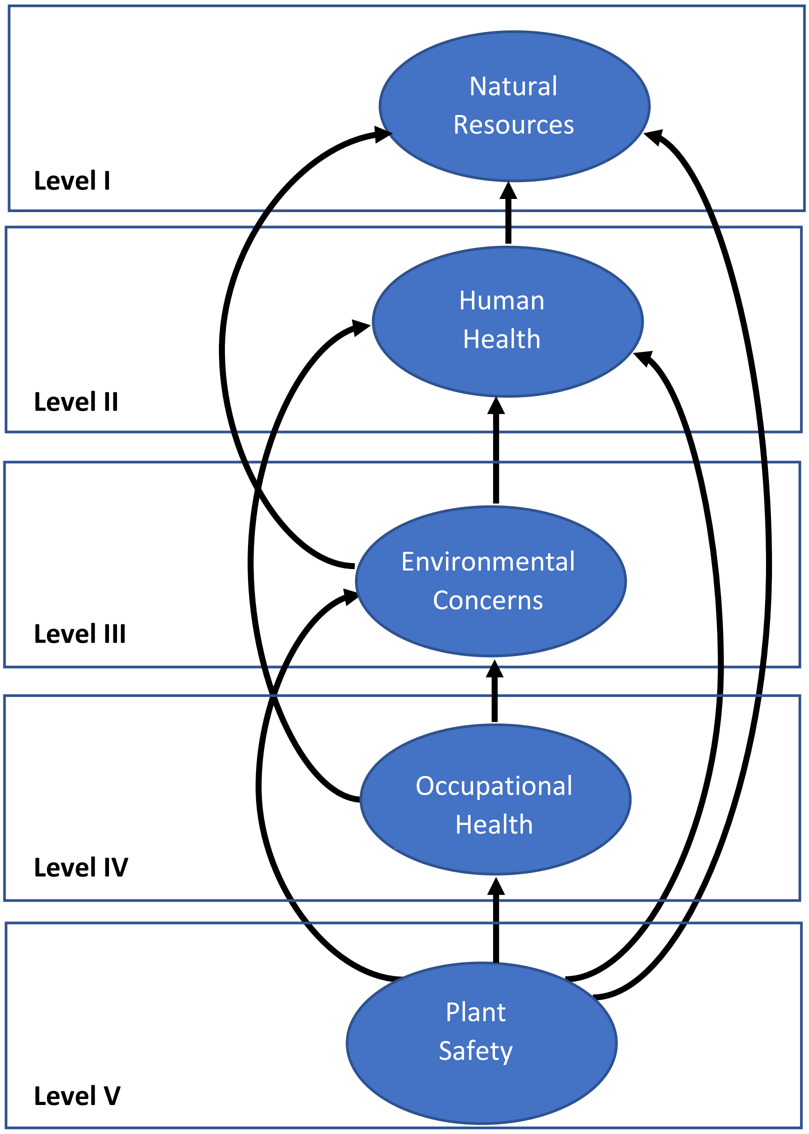


Figure 4.2 A level diagram for biodiesel performance risk factors

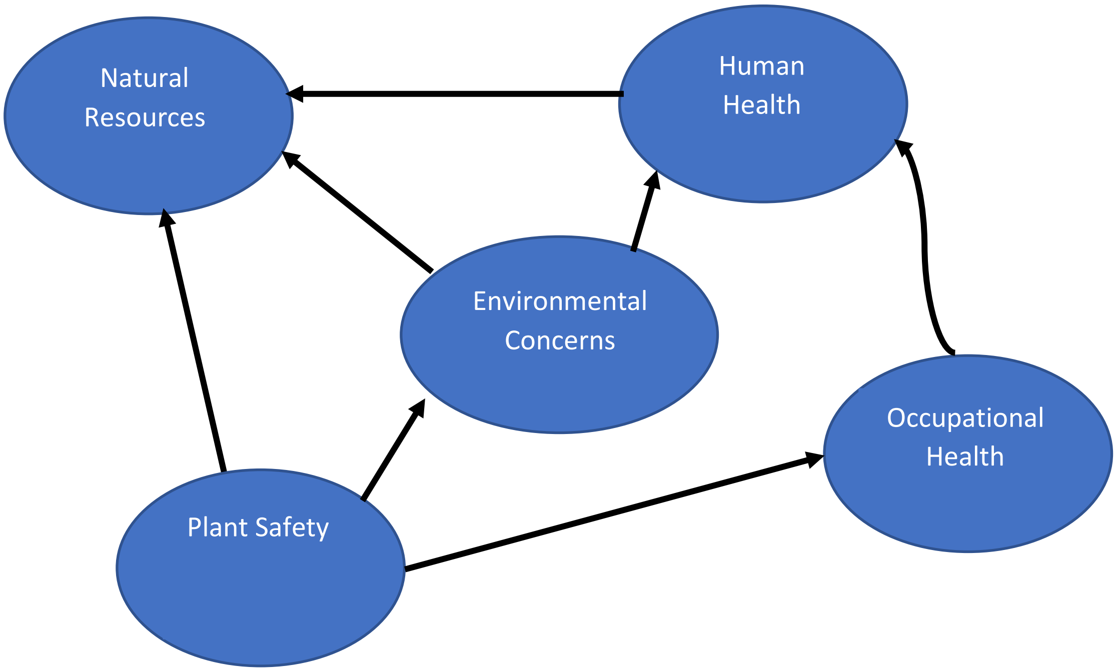
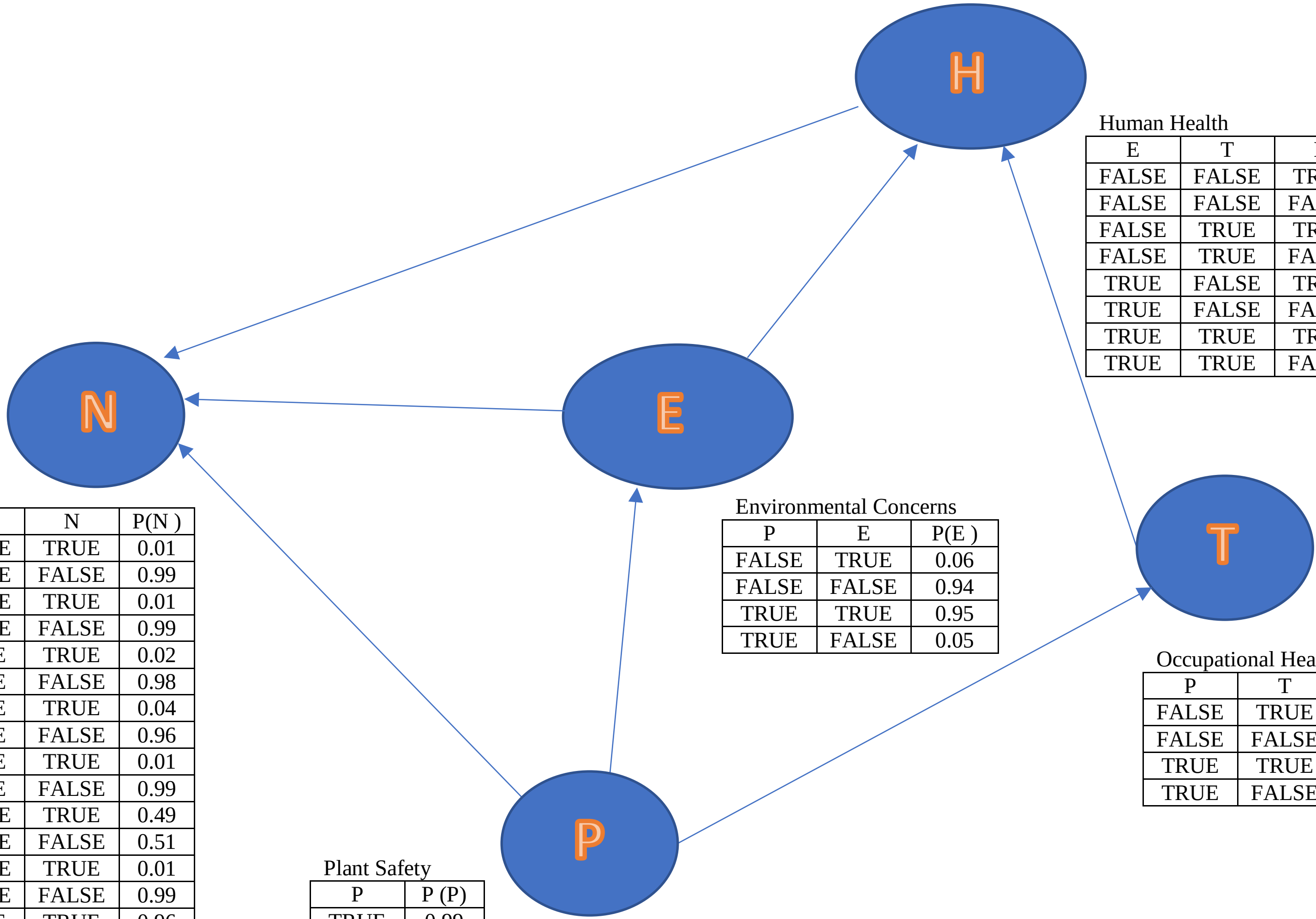


Figure 4.3 Interpretive structure model of BN based on ISM

The levels of risk factors are important in the study of the performance of a biodiesel system. From Figure 4.3 it is observed that plant safety has the highest driving power and the least dependence power. It is therefore affecting three risk factors, namely natural resources, environmental concerns and occupational health. Therefore, it can be treated as a key biodiesel performance factor and needs careful attention when biodiesel is produced. The risk factor of the natural resources category has the least driving power and a higher dependence power. This indicates that the natural resource is being affected by other risk factors but is not affecting other factors itself. The study shows that the natural resource (N) risk factor is being affected by three risk factors, namely plant safety (P), environmental concerns (E) and human health (H). The environmental concerns risk factor is affecting two risk factors, i.e., natural resources and human health, whereas it is being affected merely by plant safety. It can be observed that all risk factors are important, though some of them have more links to others. As is apparent from Figure 4.3, the natural resources (N) and human health (H) risk factors are the most influenced by the remaining risk factors, whereas plant safety is not being affected by any other risk factor. In the next phase, conditional dependency is discussed using the BN approach. As explained in the methodology section, the strength of the relation between the occurrence of occupational health (T) and natural resources (N) was studied. Figure 4.4 shows the BN along with CPTs for respective risk factors. The BN analysis provides the effect of the occurrence of occupational health on natural resources and on a whole network.



Human Health

E	T	H	P(H)
FALSE	FALSE	TRUE	0.01
FALSE	FALSE	FALSE	0.99
FALSE	TRUE	TRUE	0.71
FALSE	TRUE	FALSE	0.29
TRUE	FALSE	TRUE	0.71
TRUE	FALSE	FALSE	0.29
TRUE	TRUE	TRUE	0.95
TRUE	TRUE	FALSE	0.05

Natural Resources

P	E	H	N	P(N)
TRUE	FALSE	FALSE	TRUE	0.01
TRUE	FALSE	FALSE	FALSE	0.99
TRUE	TRUE	FALSE	TRUE	0.01
TRUE	TRUE	FALSE	FALSE	0.99
TRUE	FALSE	TRUE	TRUE	0.02
TRUE	FALSE	TRUE	FALSE	0.98
FALSE	TRUE	TRUE	TRUE	0.04
FALSE	TRUE	TRUE	FALSE	0.96
FALSE	FALSE	TRUE	TRUE	0.01
FALSE	FALSE	TRUE	FALSE	0.99
FALSE	TRUE	FALSE	TRUE	0.49
FALSE	TRUE	FALSE	FALSE	0.51
FALSE	FALSE	FALSE	TRUE	0.01
FALSE	FALSE	FALSE	FALSE	0.99
TRUE	TRUE	TRUE	TRUE	0.96
TRUE	TRUE	TRUE	FALSE	0.04

Environmental Concerns

P	E	P(E)
FALSE	TRUE	0.06
FALSE	FALSE	0.94
TRUE	TRUE	0.95
TRUE	FALSE	0.05

Occupational Health

P	T	P(T)
FALSE	TRUE	0.09
FALSE	FALSE	0.91
TRUE	TRUE	0.90
TRUE	FALSE	0.10

Plant Safety

P	P (P)
TRUE	0.99
FALSE	0.01

Figure 4.4 Conditional probability table (CPT) for Bayesian network (BN)

The results of f1 were obtained by considering all possible values of P (15 different scenarios) and are shown in Table 4.8.

Table 4.8 BN probability factor (f1) for plant safety

P	**N**	**E**	**(+T)**	**f**	**N**	**E**	**(+T)**	**f1**
T	T	T	T	2.56×10^{-3}	T	T	T	2.56×10^{-3}
T	T	F	T	8.99×10^{-5}	T	T	F	9.97×10^{-1}
T	T	F	F		T	F	T	9.08×10^{-5}
T	F	T	T	8.52×10^{-1}	T	F	F	
T	F	T	F		F	T	T	8.52×10^{-1}
T	F	F	T	4.46×10^{-2}	F	T	F	1.48×10^{-1}
T	F	F	F		F	F	T	4.47×10^{-2}
F	T	T	T	2.16×10^{-8}	F	F	F	
F	T	T	F					
F	T	F	T	8.46×10^{-7}				
F	T	F	F					
F	F	T	T	5.38×10^{-6}				
F	F	T	F					
F	F	F	T	8.45×10^{-5}				
F	F	F	F					

The results show that there is a least conditional probability (8.99×10^{-5}) of occurrence of occupational health based on non-occurrence of environmental concerns. This is true, since in the DAG, there is no direct or indirect relationship between occupational health and environmental concerns. This indicates a weak relation between the two risk factors. The occurrence probability of plant safety has the highest impact (probability of 2.56×10^{-3} or 4.46×10^{-2}) on the risk factor of occupational health for either the simultaneous occurrence or non-occurrence of natural resources and environmental concerns risk factors. This indicates a strong relationship between the plant safety and occupational health risk factors.

The results of f2 are shown in Table 4.9.

Table 4.9 BN probability factor (f2) for environmental concerns

E	T	H	P(H)	F	T	H	f2
F	F	T	0.01		T	T	0.84
F	F	F	0.99		T	F	0.05
F	T	T	0.71	0.03	F	T	
F	T	F	0.29	0.01	F	F	
T	F	T	0.71	0.81			
T	F	F	0.29				
T	T	T	0.95	0.82			
T	T	F	0.05	0.04			

The results indicate that the occurrence of environmental concerns and occupational health have the highest impact (probability of occurrence 0.82) on the occurrence of human health. However, non-occurrence of environmental concerns and occurrence of occupational health reduce the probability of occurrence of human health (probability of occurrence 0.03). Non-occurrence of occupational health and occurrence of environmental concerns gives a higher probability of human health occurrence (probability of occurrence 0.81). This indicates human health is strongly dependent on environmental concerns and that there is a weak relation between human health and occupational health.

Table 4.10 Quantitative relationship between natural resources and occupational health

H	P(N, +T)	H	P(N/+T)
F	0.06	F	0.06
T	0.84	T	0.94

The analysis in Table 4.10 shows that there exists a strong relationship between natural resources and occupational health for the occurrence of human health. The probability of occurrence is 0.94. However, the interdependency between natural resources and occupational health is weak when the impact of human health is neglected.

4.5 Conclusions and recommendations

In this work, ISM is implemented to uncover risk interdependencies of a biodiesel system performance. As a case study, operational risk factors associated with environmental, health and safety risk categories are studied. The ISM helped make rational decisions. Experts' opinions are used here as an input to construct a pairwise relationship between risk factors. The BN approach is used to study the strength of dependence and for risk analysis. It is concluded that plant safety has the highest driving power and the least dependence power and therefore it is a key risk factor, while natural resources depletion, having the least driving power and a higher dependence power, is being affected by three other risk factors. In the network analysis, it is observed that natural resources depletion is not affecting any other risk factor. The use of BN helps to understand the strength of one risk factor with other risk factors or with a whole network. The results show that occupational health has a positive impact on natural resources depletion and this relation is strongly dependent on environmental concerns. In network analysis, plant safety plays a key role and is a key biodiesel performance factor.

The analysis also indicates that the strength of the relationship between natural resources depletion and occupational health is strongly dependent on human health. It is also concluded that there exists a strong relation between plant safety and occupational health. The impact of human health on natural resources depletion cannot be ignored. The results of the strength relationship study help decision-makers in developing strategies to mitigate risks in a biodiesel system and to improve its performance. The model developed by integrating ISM and BN provides the conditional probability dependencies of a biodiesel performance system. This model could assist biodiesel production managers in effectively allocating the resources to best mange the risks. In the present work, as a case study, only one risk category has been used to show methodology applicability. However, it is recommended to apply this research methodology to other risk categories and risk factors identified in the paper. In addition, future research should consider economic and environmental risk factors to study overall biodiesel performance analysis. This would help to develop a green, safe, and economical biodiesel production system.

4.6 References

Achten, W. M. J., L. Verchot, Y. J. Franken, E. Mathijs, V. P. Singh, R. Aerts and B. Muys (2008). "Jatropha bio-diesel production and use." Biomass and Bioenergy 32(12): 1063-1084.

Apostolakou, A. A., I. K. Kookos, C. Marazioti and K. C. Angelopoulos (2009). "Techno-economic analysis of a biodiesel production process from vegetable oils." Fuel Processing Technology 90(7–8): 1023-1031.

Atabani, A. E., A. S. Silitonga, H. C. Ong, T. M. I. Mahlia, H. H. Masjuki, I. A. Badruddin and H. Fayaz (2013). "Non-edible vegetable oils: A critical evaluation of oil extraction, fatty acid compositions, biodiesel production, characteristics, engine performance and emissions production." Renewable and Sustainable Energy Reviews 18: 211-245.

Attri, R., S. Grover, N. Dev and D. Kumar (2012). "An ISM approach for modelling the enablers in the implementation of Total Productive Maintenance (TPM)." International Journal of System Assurance Engineering and Management 4(4): 313-326.

Azeem, M. W., M. A. Hanif, J. N. Al-Sabahi, A. A. Khan, S. Naz and A. Ijaz (2016). "Production of biodiesel from low priced, renewable and abundant date seed oil." Renewable Energy 86: 124-132.

Cameron, I. T. and R. Raman (2005). Process Systems Risk Management, Elsevier Science.

Chidambaranathan, S., C. Muralidharan and S. G. Deshmukh (2008). "Analyzing the interaction of critical factors of supplier development using Interpretive

Structural Modeling—an empirical study." The International Journal of Advanced Manufacturing Technology 43(11): 1081-1093.

Christopher, M., C. Mena, O. Khan and O. Yurt (2011). "Approaches to managing global sourcing risk." Supply Chain Management: An International Journal 16(2): 67-81.

Czuchry, A. J. and M. M. Yasin (2003). "Managing the project management process." Industrial Management & Data Systems 103(1): 39-46.

Demirbas, A. and M. F. Demirbas (2010). Algae Energy: Algae as a New Source of Biodiesel, Springer London.

Fu, Q., C. Song, Y. Kansha, Y. Liu, M. Ishizuka and A. Tsutsumi (2015). "Energy saving in a biodiesel production process based on self-heat recuperation technology." Chemical Engineering Journal 278: 556-562.

Govindan, K., S. G. Azevedo, H. Carvalho and V. Cruz-Machado (2015). "Lean, green and resilient practices influence on supply chain performance: interpretive structural modeling approach." International Journal of Environmental Science and Technology 12(1): 15-34.

Guldhe, A., P. Singh, S. Kumari, I. Rawat, K. Permaul and F. Bux (2016). "Biodiesel synthesis from microalgae using immobilized Aspergillus niger whole cell lipase biocatalyst." Renewable Energy 85: 1002-1010.

Haas, M. J., A. J. McAloon, W. C. Yee and T. A. Foglia (2006). "A process model to estimate biodiesel production costs." Bioresource Technology 97(4): 671-678.

Jallow, A. K., B. Majeed, K. Vergidis, A. Tiwari and R. Roy (2007). "Operational risk analysis in business processes." BT Technology Journal 25(1): 168-177.

Jensen, F. V. (1996). An introduction to Bayesian networks, UCL Press London.

Kim, S. and B. E. Dale (2005). "Life cycle assessment of various cropping systems utilized for producing biofuels: Bioethanol and biodiesel." Biomass and Bioenergy 29(6): 426-439.

Lardon, L., A. Hélias, B. Sialve, J.-P. Steyer and O. Bernard (2009). "Life-Cycle Assessment of Biodiesel Production from Microalgae." Environmental Science & Technology 43(17): 6475-6481.

Lockamy, A. and K. McCormack (2012). "Modeling supplier risks using Bayesian networks." Industrial Management & Data Systems 112(2): 313-333.

Mandal, A. and S. G. Deshmukh (1994). "Vendor Selection Using Interpretive Structural Modelling (ISM)." International Journal of Operations & Production Management 14(6): 52-59.

Marulanda, V. F. (2012). "Biodiesel production by supercritical methanol transesterification: process simulation and potential environmental impact assessment." Journal of Cleaner Production 33: 109-116.

Nair, S. (2011). IDENTIFYING AND MANAGING PROCESS RISKS RELATED TO BIOFUEL PROJECTS AND PLANTS. Hazards Xxii: Process Safety and Environmental Protection. Rugby, Inst Chemical Engineers: 331-338.

Pai, R. R., V. R. Kallepalli, R. J. Caudill and Z. MengChu (2003). Methods toward supply chain risk analysis. IEEE International Conference on Systems, Man and Cybernetics, 2003.

Pfohl, H. C., P. Gallus and D. Thomas (2011). "Interpretive structural modeling of supply chain risks." International Journal of Physical Distribution & Logistics Management 41(9): 839-859.

Sajid, Z., F. Khan and Y. Zhang (2016). "Process simulation and life cycle analysis of biodiesel production." Renewable Energy 85: 945-952.

Sajid, Z., Y. Zhang and F. Khan (2016). "Process design and probabilistic economic risk analysis of bio-diesel production." Sustainable Production and Consumption 5: 1-15.

Salzano, E., M. Di Serio and E. Santacesaria (2010). "Emerging Risks in the Biodiesel Production by Transesterification of Virgin and Renewable Oils." Energy & Fuels 24(11): 6103-6109.

Singh, M. D. and R. Kant (2008). "Knowledge management barriers: An interpretive structural modeling approach." International Journal of Management Science and Engineering Management 3(2): 141-150.

Srinivas, D. and J. K. Satyarthi (2010). "Biodiesel Production from Vegetable Oils and Animal Fat over Solid Acid Double-Metal Cyanide Catalysts." Catalysis Surveys from Asia 15(3): 145-160.

Trucco, P., E. Cagno, F. Ruggeri and O. Grande (2008). "A Bayesian Belief Network modelling of organisational factors in risk analysis: A case study in maritime transportation." Reliability Engineering & System Safety 93(6): 845-856.

van Kasteren, J. M. N. and A. P. Nisworo (2007). "A process model to estimate the cost of industrial scale biodiesel production from waste cooking oil by supercritical transesterification." Resources, Conservation and Recycling 50(4): 442-458.

Wang, J. M., Y. M. Li and Y. P. Zhu (2014). The Interpretive Structural Model of EPC Project Risk Factors. Applied Mechanics and Materials, Trans Tech Publ.

Warfield, J. N. (1974). "Developing Interconnection Matrices in Structural Modeling." IEEE Transactions on Systems, Man and Cybernetics SMC-4(1): 81-87.

Weber, P., G. Medina-Oliva, C. Simon and B. Iung (2012). "Overview on Bayesian networks applications for dependability, risk analysis and maintenance areas." Engineering Applications of Artificial Intelligence 25(4): 671-682.

Williams, P. R. D., D. Inman, A. Aden and G. A. Heath (2009). "Environmental and Sustainability Factors Associated With Next-Generation Biofuels in the U.S.: What Do We Really Know?" Environmental Science & Technology 43(13): 4763-4775.

Zhi, H. (1995). "Risk management for overseas construction projects." International Journal of Project Management 13(4): 231-237.

Chapter 5

5 A novel process economic risk model

Authorship and contributorship

This work has been written as a manuscript by Sajid, Z., Khan, F., & Zhang, Y. (2017). “A novel process economic risk model”. The work has been submitted to a journal for publication. The first author, Zaman Sajid, formulated the research problem. The developed research problem was critically reviewed by co-author, Dr. Faisal Khan. The first author performed the analysis, executed the case study and drafted the manuscript. The co-author, Dr. Faisal Khan, critically reviewed the developed approach and provided feedback to improve it throughout the project. The co-authors, Drs. Yan Zhang & Faisal Khan further reviewed the developed approach and provided feedback to improve the approach, the presentation of the results and the manuscript as a whole.

Abstract

In this paper, the concept of value at risk (VaR) is introduced to study process economics related to biodiesel production and use. Although the VaR concept is actively used in financial engineering for stock investment and trading, it has never been used in process economics. A methodology to develop a VaR model for a biodiesel process facility has been proposed and analysed. The impact of different cost related risk factors was modelled using stochastic process and interdependence in a Bayesian Network formalism. The analysis revealed that cost underestimation was the most significant risk factor in biodiesel economics. The VaR model was analysed for 1, 5, and 10 VaR up to 5 years of plant operations. Analysing VaR at any point of time (i.e. year 2) showed that with a 1% chance, 5% chance and 10% chance, the maximum loss would be \$6.26, \$9.52 and \$11.34 million respectively (up to year 2). When VaR is considered in the process economics the return period is significantly affected and is increased by 21 months. This study recommends that VaR should be considered as an integral part of process economics, especially for new product or process design.

5.1 Introduction

In a process industry, financial risk management plays a key role to identify risk sources, measure their economic impact and propose the ways to manage exposure to such risks in an economical way. The overall objective of financial risk management is to assess, manage and control the risk associated with profit or return. To build and operate a large biodiesel production plant there is a need for careful financial risk quantification since the investment is in billions of dollars and investors want to know the level of risk associated with returns. In 2005, Biofuels Corporation PLC, while seeking to establish one of Europe's largest biodiesel plants in Teesside, England, declared to have an additional £33 million when construction went into cost overrun (Shah 2005). This unexpected cost escalation was due to many factors, which altered the total cost and affected the profit and payback period. This is a common story for many large projects, and highlights a need to study the impact of biodiesel cost related risk factors on the total cost of biodiesel production and the risk calculations associated with returns.

In recent decades, biodiesel has emerged as an environmentally friendly biofuel and as an appropriate replacement for conventional petroleum based diesel fuel. On an industrial scale, biodiesel is produced by a chemical reaction of biomass and alcohol in the presence of a catalyst. The reaction is known as the trans-esterification reaction. Depending on reaction kinetics, the alcohol could be methanol or ethanol and the catalyst could be acidic, alkaline or enzymatic (Balat and Balat 2010). Biomass comes in different materials. These are edible sources, non-edible sources, algae biomass and microscopic organisms. The edible sources include corn, sugarcane, sugar beet, wheat, barley, rapeseed, soybean, potato, animal fats and vegetable oils (Gerpen 2005, Kinney and Clemente 2005). The non-edible sources include grass, municipal solid waste, wood, sewage sludge, jatropha oil, agriculture, forest residues and others (Banković-Ilić, Stamenković et al. 2012, Atabani, Silitonga et al. 2013). Research is also being conducted to produce biofuel from algae as biomass (Sambusiti, Bellucci et al. 2015, Ullah, Ahmad et al. 2015). Genetically modified microbes are being used to produce biofuels, which include cyanobacteria, fungi, yeast and microalgae (Vassilev and Vassileva 2016).

The commercialization of biodiesel necessitates process economics and a life cycle assessment study of biodiesel production using the aforementioned biomass feedstocks. The process economics of industrial scale production of biodiesel using different biomasses and technologies is under study (Chen, Zhou et al. 2015, Eguchi, Kagawa et al. 2015, Formighieri 2015, Sajid, Zhang et al. 2016, Wu, Wei et al. 2016). Research is also being conducted to study the life cycle impact of biodiesel usage from various biomasses (Fasahati, Woo et al. 2015, Sajid, Khan et al. 2016b). As many large-scale production aspects of biodiesel production using different raw materials are in the early stages of investigation, financial risk quantification is a big challenge and so are their management and the mitigation of risk sources.

Value at risk (VaR) is a new statistical term being used to diagnose risk exposure in financial risk quantification. VaR represents the threshold or maximum expected loss on an asset or return which could happen over a certain time period with a given confidence interval (J. and D. 2000). The advantage of using VaR lies in the fact that it summarises the worst expected loss due to all quantifiable risks associated with an investment as a single number (Bohdalová 2007). The probability distributions of earnings or losses of an investment are used to describe VaR. The inclusive confidence level is provided by specifying the probability level in the probability distribution profile of the possible gains of an investment over a given time period. In finance, VaR is typically calculated using three approaches: a nonparametric approach (historical method), parametric approach and Monte Carlo Simulation (Culp 2002; Jorion 2006; Sadeghi and Shavvalpour 2006; Cakir and Uyar 2013).

The modelling of VaR using nonparametric methods was shown by Cheung and Powell (2012). In their subsequent work, they demonstrated VaR modelling using a parametric method and Monte Carlo Simulation (Cheung and Powell 2013). They developed a methodology to perform VaR calculations in Microsoft® Excel for a single asset and a portfolio. In their analysis, they considered return on the price of the share as a risk factor. Though their work was a significant initiative to compute VaR using an inexpensive approach, there are some limitations with their methodologies. In their Excel modelling, they fixed the numbers of observations (2512 in nonparametric methodology) and the numbers of trials (2000 in Monte Carlo Simulation methodology). In Excel, they developed all formulas based on these fixed numbers of observations or trials. However, in Excel, it is quite a tedious job to alter all the formulas if one wishes to change the number of observations or trials. Moreover, in Monte Carlo Simulation, there is a need to achieve stability of the solution by taking enough samples (around 10,000 iterations). In their model, they used Excel, and it is hard to implement such stability beyond 2000 iterations in Excel. Moreover, they used pseudo-random numbers to generate random numbers. Though this allowed them to re-examine their simulation results, this does not create stability in the results which means there should not be any change in the results by changing the number of samples and iterations.

Another methodology to quantify VaR was presented by Beneda (2005) as part of a study in which the author quantified and optimised the overall risk of an asset management firm using computerised simulation. The work studied four risk categories which a firm may face. These included operational risks, strategic risks, pure risks and financial risk. The author used the Monte Carlo Simulation approach by sampling experiments to estimate the distribution of after-tax operating income and analysed the profile to calculate VaR. The outcome variable (after-tax operating income) was modelled based on different probabilistic inputs of the four risk factors. Though the results provided a deterministic model to compute VaR based on after-tax operating income the study does not provide any mutual inter-dependency among the risk factors studied. This means the study does not provide VaR based on the inter-relationship among operational risks, strategic risks, pure risks and financial risks, since these risk factors are highly dependent on each other.

In another work, Olson and Wu (2010) presented VaR computations using three different approaches and presented a simulation process for Monte Carlo Simulation to compute VaR. They presented a five-step methodology to perform their simulation process. Their simulation process was done using Crystal Ball software. They demonstrated VaR simulation by considering the Monte Carlo Simulation model presented by Beneda (2005). Their resulting explanations were helpful to understand the VaR computations; however, the work does not discuss the impact of each individual risk factor on either operating income or after-tax income.

As is evident from the previous studies, VaR has been used in limited number cases, due to lack of understanding of risk factors, their interaction and dependency on the overall system's performance (profit). This work is planned with the following objectives: i) to identify key risk factors related to the engineering system and develop a risk model that represents the interaction and dependency of these risk factors, and ii) to use the developed risk model to study the value of the risk for different scenarios and estimate overall profitability. The applicability of the methodology and the VaR concept is demonstrated using a biodiesel production system as a test case.

This work will open a new dimension in process economics and will help build a robust financial model. These models will be useful for early project cost and insurance estimation.

5.2 Methodology

5.2.1 Considerations

The inter-dependent total cost estimation and VaR analysis are based on the following assumptions:

- The VaR analysis was conducted on risks associated with returns of a biodiesel production plant. All monetary values are reported in US dollars.
- On an annual basis, the plant production capacity is 45,000 tonnes of biodiesel. Biodiesel has a high market demand and all produced biodiesel can be sold.
- Only quantifiable financial risks were used to compute VaR.
- Only risk factors associated with cost estimation were considered. The risk associated with revenue (biodiesel market risks, biodiesel demand and supply risks and others) was not considered in this study.
- Total cost is an uncertain variable and its value is influenced by cost related risk factors, which subsequently influence the profit.
- Biodiesel raw materials logistic risks were not considered in this study.

- The biodiesel economic analysis along with all assumptions presented by Sajid and co-researchers (2016) are valid for this study and the cost as well as their revenue data were used in this study. The cost data were updated to year 2016 using Chemical Engineering Plant Cost Index (CEPCI). The CEPCI for year 2016 is 540.9 (June 2016) (Lozowski 2016).
- The time value of money was included using 5% annual interest and inflation rates.
- The relationship between the total cost and cost related risk factors was assumed to be linear.

5.2.2 Methodology Description

The proposed process economics methodology comprises six major steps. To demonstrate each step, a simple example of a water bottle manufacturing unit is used. The steps in this methodology are:

Step 1: Process economics model

The purpose of this step was to estimate the total cost of production, the revenue and the profit earned by selling the products produced from the production facility. The process economic model of various products has been well presented in the literature (Ofori-Boateng and Lee 2011; Renda, Gigli et al. 2016; Sajid, Zhang et al. 2016). For the current example, it was considered that the total cost of production was \$2, \$2.4, \$2.8, \$3.2, and \$3.6 for years 1, 2, 3, 4, and 5 respectively. The bottles were sold for \$12, \$12.7, \$13.4, \$14.1, and \$14.8 in respective years.

Step 2: Identification of cost related risk factors

The goal of this step was to enlist all cost related risk factors and then select the most important ones for the process economics model. Cost related risk factors were determined based on a detailed literature review. For the water bottle manufacturing unit, the cost related risk factors considered were: i) transportation cost of raw materials ii) cost of labour, and iii) budget availability.

Step 3: Qualitative interdependency study of cost risk factors

The goal of this step was to perform a qualitative interdependency study of cost related risk factors, identified in step 2. The cost related risk factors were correlated using Interpretive Structural Modelling (ISM) (Colin, Estampe et al. 2011; Venkatesh, Rathi et al. 2015; Sajid, Khan et al. 2016a). The purpose of this step was to transform complex, poorly articulated, unclear and unstructured inter-relationship information of cost related risk factors into well-articulated, clearly communicated and structured information. The results were represented in terms of visual mapping of the correlation of cost related risk factors. This step helped to visualize their interdependence. The inputs for this step were expert's opinions, which developed a structural self-interaction matrix. The matrix consisted of a pairwise comparison of risk factors (Sajid, Khan et al. 2016a). The ISM developed for the bottle-manufacturing unit is shown in Figure 5.1.

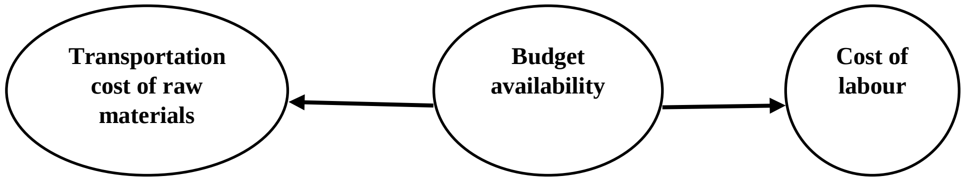
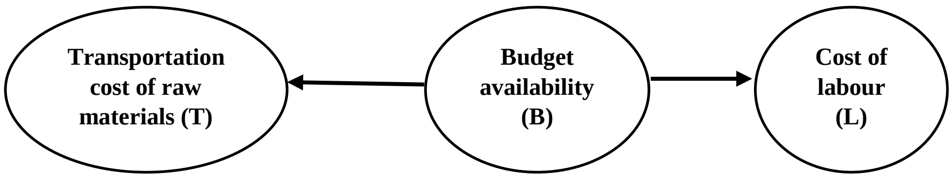


Figure 5.1 Interpretive Structural Model (ISM) for bottle manufacturing unit

This shows that budget availability influences both transportation cost of raw materials and cost of labour.

Step 4: Quantitative interdependency study of cost risk factors

The qualitative relationships developed among cost risk factors were transformed into quantitative ones by applying the Bayesian Network (BN) approach. The purpose of this step was to evaluate the strength of the relationship among cost related risk factors and the objective was achieved through BN approach (Sajid, Khan et al. 2016a). Expert opinion was used to allocate an initial quantitative relation among risk factors by developing conditional probability tables (CPT) and marginal probabilities for the nodes. For a current example of a bottle manufacturing unit, the CPT for the network in step 3 is shown in Figure 5.2.



B	P(T)
T	0.7
F	0.4

P(B)
0.9

B	P(L)
T	0.8
F	0.6

Figure 5.2 Conditional probability table (CPT) for bottle manufacturing unit

Using the variable elimination method, Table 5.1 was constructed. The methodology has been represented in a previous work (Sajid, Khan et al. 2016a).

Table 5.1 Variable elimination method

Cost risk factor	P(T/L) - True	P(T/L) - False
Transportation cost of raw materials	0.78	0.22
Budget availability	0.80	0.20

Cost of labour	0.67	0.33

Step 5: Screening of significant and insignificant cost risk factors

In this step, cost related risk factors were screened out to exclude insignificant risk factors. A linear model was developed using linear function to approximate the relationships among cost related risk factors and the total cost of the process economic study (step 1). A statistical tool, multiple regression analysis, was used to develop this model. Previously, various researchers have used this concept in other fields (Bandara and Dassanayake 2006; Farooq, Ishaq et al. 2013; Chatterjee and Hadi 2015) and it was implemented on a process facility in this work. The predictors in the regression model were cost related risk factors and the response variable was the total cost. In this categorical analysis, the predictors were assigned dummy variables and the impact on the outcome variable (total cost) was noticed. Dummy variables were represented by either the existence or non-existence of the risk factors (events). The quantitative values for the existence of events were adopted from BN analysis in step 4. The non-existence was assigned a zero value. A risk matrix, consisting of the combination of existence or non-existence of events, was developed to perform multiple regression analysis. The multiple regression analysis was performed in Microsoft® Excel. A multi-collinearity test was performed using Excel correlation analysis before performing regression analysis. However, regression results could be interpreted in the presence of multi-collinearity, as has been discussed by various researchers (Zou, Tuncali et al. 2003; Kraha, Turner et al. 2012; Nimon and Oswald 2013). A variable was considered statistically significant if both its p-value and significance F value were less than 0.05; otherwise, it was rejected. The multiple regression analysis was performed until the best model (as per p-value and significance F criteria) was obtained.

For the current example of the bottle manufacturing unit, the model was

$Y = \beta_0 + \beta_T X_T + \beta_B X_B + \beta_L X_L$

where, Y = total cost in dollars (estimated from process economics)

β_0 = y-intercept of the total cost

X_T, X_B, X_L were predictors for the transportation cost of raw materials, budget availability and cost of labour respectively. β_T, β_B, ,β_L were the regression coefficients of the transportation cost of raw materials, budget availability and cost of labour respectively. The regression analysis indicated that transportation cost and budget availability were the only significant variables with β_T and β_B of -12.30 and -6 respectively. The analysis had the adjusted R square value of 0.88 and a standard error of 1.44. The intercept was 13.8. The regression model showed that for a unit dollar of each cost risk factor, the total cost was calculated as less than \$4.5 and therefore the actual total cost for year 1 was \$6.50. With an updated value of actual total costs for each year, the process economic model was updated accordingly.

Step 6: Value at Risk (VaR) analysis and results interpretation

In this step, Monte Carlo Simulation was performed on an updated process economic model, obtained from step 5, with using Oracle® Crystal Ball software. The probabilistic input variables were total cost and revenue while the outcome variable was the profit. Probabilistic input variables were assigned normal distributions in Crystal Ball while profit was defined as forecast value. The simulation was performed for 10,000 iterations and the result was a probability distribution profile for profit. The profit profile was analysed for 99%, 95% and 90% confidence and value at risk (VaR) was reported. The analysis was performed for years 1, 2, 3, 4 and 5 and the impact of the cost related risk factor was analysed to determine the payback period affected. To elaborate this step using the water bottle manufacturing example, normal distribution was assigned to the actual cost, with a mean of 6.50 and a standard deviation of 0.65 for a total cost of \$6.50. The normal distribution was assigned to revenue having a mean of 12.00 and standard deviation of 1.20 for a revenue value of \$12.00. The results show that for year 1, 1 VaR was \$2.26, 5 VaR was \$3.26 and 10 VaR was \$3.74. The results of VaR are interpreted as, for 1 VaR, there is a 1% chance that the profit will fall to \$2.26 or below in the time period of year 1 or that there is a 99% chance that the profit of a bottle manufacturing investor will not fall below \$2.26 in year 1. The 5 VaR shows that there is a 5% chance that the profit loss will be \$3.26 or less in the same year. In the case of 10 VaR, profit loss falling to \$3.74 or less has a 10% chance in the same year. A similar procedure was repeated for subsequent years.

5.3 Application: Process Economics Analysis for a biodiesel production plant

In this section, the methodology proposed above has been implemented on a biodiesel production plant. The biodiesel production plant is producing biodiesel using an alkali-catalysed process. The biomass feedstock is non-edible jatropha oil.

Step 1: Process economics model

The biomass feedstock conversion to biodiesel, its process flow diagram (PFD) and an economic analysis of a biodiesel plant for a given capacity of a plant have been presented in a previous publication (Sajid, Zhang et al. 2016) and the results were used in this study. The data collected from their work was total cost and revenue. The economic data was updated to the current year, 2016.

Step 2: Identification of cost related risk factors

Detailed research was conducted and a list of biodiesel cost related risk factors were presented in previous work (Sajid, Khan et al. 2016a). Three categories of cost related risk factors were presented. These were risk related to the process category, risk related to design and installation and risk related to the operation category. In this work, the risk factors in a sub-category of process named costs were chosen to study extensively. The cost related risk factors chosen in this study were cost underestimation, contingency cost, cost overrun, budget conformity and financial exposition.

Step 3: Qualitative interdependency study of cost risk factors

A structural self-interaction matrix was developed by using expert inputs in pairwise comparison bases as shown in Table 5.2. A matrix was developed in Microsoft Excel and an expert was asked to provide his opinion based on three categories. The responses were "yes", if a dependency exists; "no", if dependency does not exist and "not related" if he thinks no relation exists between the two. Using the ISM technique discussed in (Sajid, Khan et al. 2016a), an ISM based model for cost related risk factors was developed which provided visual mapping of correlations among cost related risk factors.

Table 5.2 SSIM for step 3

	Cost overrun	Cost underestimation	Budget conformity	Financial exposition	Contingency cost
Cost overrun		Y	Y	N	Y
Cost underestimation	Y		N	N	N
Budget conformity	Y	Y		N	Y
Financial exposition	N	Y	Y		Y
Contingency cost	N	N	Y	N	

Step 4: Quantitative interdependency study of cost risk factors

The expert's inputs were taken to develop CPTs and marginal probabilities for each biodiesel cost related risk factor. Using the BN approach, the variable elimination method was used to develop an algorithm and the algorithm was numerically computed.

Step 5: Screening of significant and insignificant cost risk factors

A multiple regression model was developed using Microsoft Excel to approximate the relationships among biodiesel cost risk factors and total cost, obtained from biodiesel process economics from step 1. The predictors or independent variables were biodiesel cost risk factors while their impact on the total cost (known as dependent/response variables in regression analysis) was being studied. For current analysis, the model was

$$y = \beta_0 + \beta_A X_A + \beta_C X_C + \beta_E X_E + \beta_F X_F + \beta_D X_D$$

in which, y was the total cost in millions of dollars– a response variable

β_0 = y-intercept of the total cost line

X_A, X_C, X_E, X_F and X_D were the cost related risk factors, namely, cost underestimation, contingency cost, cost overrun, financial exposition and budget conformity predictors respectively.

β_A, β_C , β_E , β_F and β_D were the parameters of respective risk factors which determine the contributions of cost underestimation, contingency cost, cost overrun, financial exposition and budget conformity predictors respectively. The matrix developed to perform multiple regression analysis in shown in Table 5.3. The matrix shows the combination of the existence or non-existence of an event in the analysis.

Table 5.3 Risk factors matrix

Cost Underestimation	**Budget conformity**	**Cost overrun**	**Financial exposition**	**Contingency cost**
Event occurs	Event does not occur	Event does not occur	Event does not occur	Event does not occur
Event does not occur	Event occurs	Event does not occur	Event does not occur	Event does not occur
Event does not occur	Event does not occur	Event occurs	Event does not occur	Event does not occur
Event does not occur	Event does not occur	Event does not occur	Event occurs	Event does not occur
Event does not occur	Event does not occur	Event does not occur	Event does not occur	Event occurs

Step 6: Value at Risk (VaR) analysis and results interpretation

The actual total cost from step 5 and revenue for each year from step 1 were assigned normal probability distributions and Monte Carlo Simulation was performed using Oracle® Crystal Ball software. The output was the cumulative probability profile of profit. The profile was analysed at 1%, 5% and 10% chances and the results of VaR were analysed.

5.4 Results and discussion

According to the biodiesel process economics and the production schedules for years 0, 1, 2, 3, 4 and 5, the total cost for each respective year is $1.25, $3.07, $18.28, $27.76, $31.07 and $34.39 million. Based on the yearly revenues of $0, $0, $43.05, $94.71, $104.18 and $114.60 million for respective years, the subsequent estimated profit for respective years is $0, $0, $24.76, $66.94, $73.10 and $80.20 million. There was no profit in years 0 and 1 due to the plant's start-up schedule; the plant started to produce and sell biodiesel from year 2. Based on the expert input, the ISM model for cost related risk factors is shown in Figure 5.3. For the purpose of simplicity and clarity some relations have been ignored in the final ISM model.

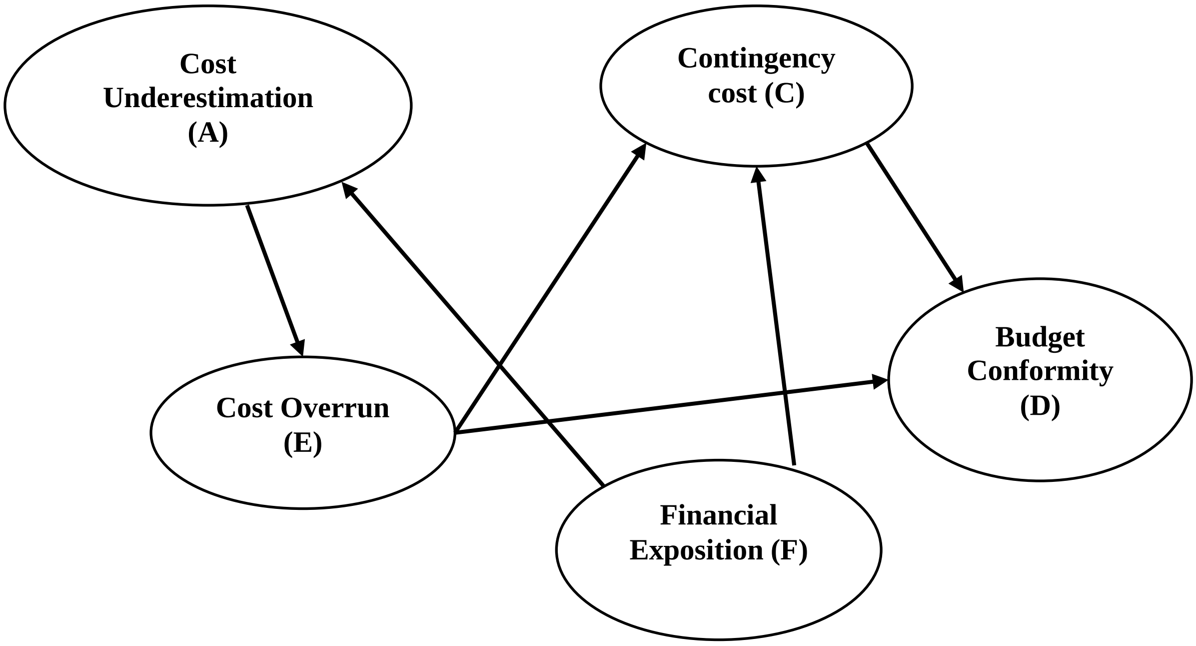


Figure 5.3 ISM model for cost related risk factors

Figure 5.3 represents the qualitative interdependency of various risk factors. This shows that cost underestimation is being influenced by financial exposition while it is influencing cost overrun. Contingency cost influences budget conformity and is influenced by two cost related risk factors, which are financial exposition and cost overrun. These qualitative relationships were converted into quantitative ones using the BN technique. The CPTs and marginal probabilities of cost underestimation (A), cost overrun (E), contingency cost (C), budget conformity (D) and financial exposition (F) are shown in Figure 5.4. In this study, the conditional probability of cost underestimation (A) given the probability of Contingency (C), P(A/C), is studied. Since the objective is to study the impact of cost performance risk factors on VaR, the probability model is analysed using the occurrence or non-occurrence of each risk factor. Using the BN approach, the algorithm developed using a variable elimination method is shown below.

The initial factors of the study are: P (A/F), P (F), P (C/E, F), P (D/C,E), P (E/A). With these, the elimination order considered is F, D and E.

For F: $f1(A, C, E, D) = \sum_{\text{All values of F}} P(F). P(A / F). P(C/E, F)$

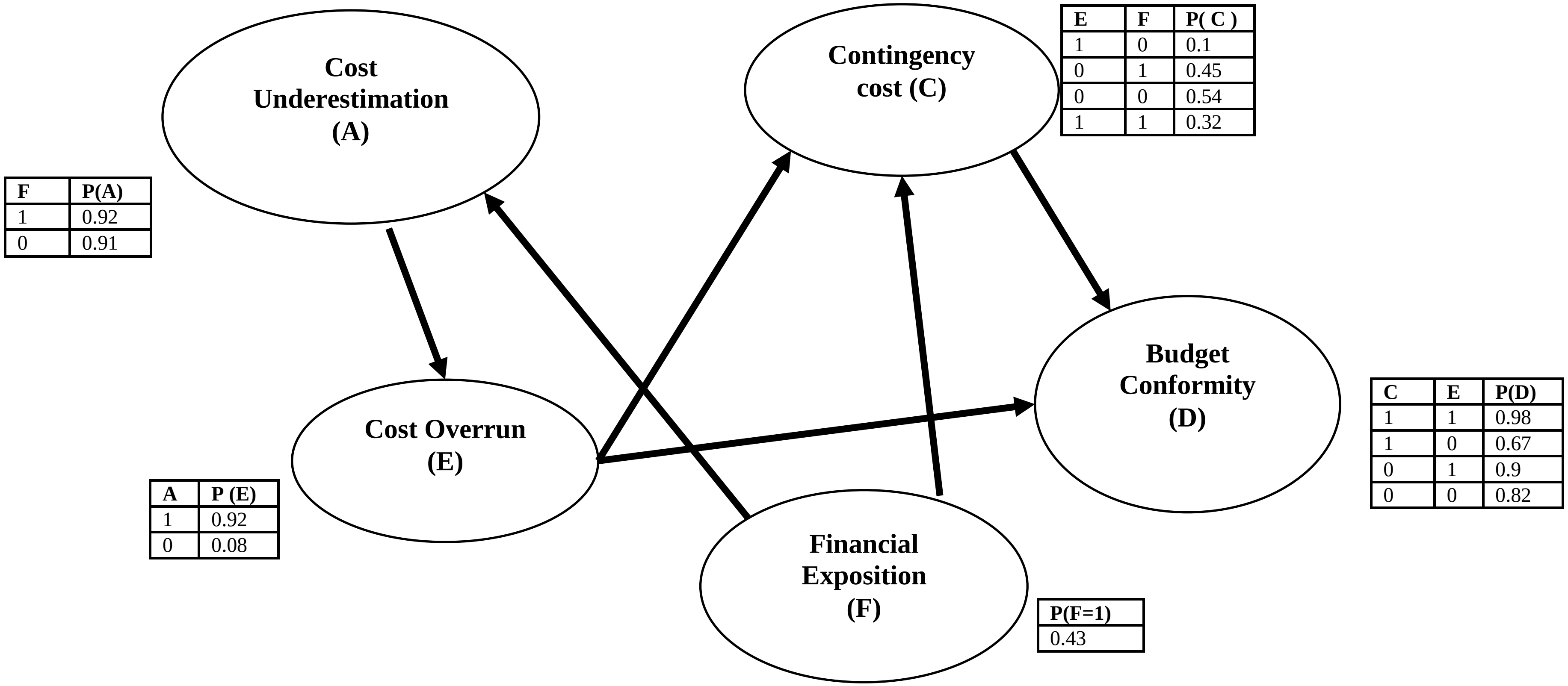
For D: $f2(A, C, E) = \sum_{\text{All values of D}} f1(A, C, E, D). P(D/C, E)$

For E: $f3(A, C) = \sum_{\text{All values of E}} f2(A, C, E). P(E/A)$

P(A, C) = f3(A, C)

Renormalization gives:

P(A/C) = P(A, C)/P(C)



F	P(A)
1	0.92
0	0.91

A	P (E)
1	0.92
0	0.08

E	F	P(C)
1	0	0.1
0	1	0.45
0	0	0.54
1	1	0.32

C	E	P(D)
1	1	0.98
1	0	0.67
0	1	0.9
0	0	0.82

P(F=1)
0.43

Figure 5.4 Expert inputs for conditional probability table (CPT) in Bayesian Network (BN) analysis

The results of the interdependency quantification using a BN approach are presented in Table 5.4.

Table 5.4 Results of BN approach

Category – P(A/C)	True	False
Cost underestimation	0.65	0.35
Contingency cost	0.55	0.45
Cost overrun	0.57	0.43
Budget conformity	0.36	0.64
Financial exposition	0.39	0.61

The results indicate that cost underestimation has the highest influence on the whole network while budget conformity has the least impact on the network, though it is a significant risk factor in the network. The results also show that after cost underestimation, cost overrun and contingency cost are influencing the whole network at second and third place respectively. The input model for regression analysis is shown in Table 5.5, where total cost was a dependent variable and risk factors were the predictors. Table 5.5 represents the probabilities of the predictors and total cost in millions of US dollars.

Table 5.5 Regression model inputs

P (cost underestimation)	P (budget conformity)	P (cost overrun)	P (financial exposition)	P (contingency cost)	Total cost ($ million)
0.65	0.00	0.00	0.00	0.00	1.26
0.65	0.00	0.00	0.00	0.00	3.08
0.65	0.00	0.00	0.00	0.00	18.28
0.65	0.00	0.00	0.00	0.00	27.76
0.65	0.00	0.00	0.00	0.00	31.08
0.00	0.36	0.00	0.00	0.00	34.40
0.00	0.36	0.00	0.00	0.00	37.71

0.00	0.36	0.00	0.00	0.00	41.03
0.00	0.36	0.00	0.00	0.00	44.35
0.00	0.36	0.00	0.00	0.00	47.66
0.00	0.00	0.57	0.00	0.00	53.38
0.00	0.00	0.57	0.00	0.00	56.04
0.00	0.00	0.57	0.00	0.00	58.85
0.00	0.00	0.57	0.00	0.00	61.79
0.00	0.00	0.57	0.00	0.00	64.05
0.00	0.00	0.00	0.39	0.00	73.22
0.00	0.00	0.00	0.39	0.00	77.54
0.00	0.00	0.00	0.39	0.00	81.85
0.00	0.00	0.00	0.39	0.00	86.16
0.00	0.00	0.00	0.39	0.00	90.48
0.00	0.00	0.00	0.00	0.55	94.79
0.00	0.00	0.00	0.00	0.55	99.10
0.00	0.00	0.00	0.00	0.55	103.42
0.00	0.00	0.00	0.00	0.55	107.73
0.00	0.00	0.00	0.00	0.55	112.04
0.35	0.00	0.00	0.00	0.00	116.36
0.35	0.00	0.00	0.00	0.00	120.67
0.35	0.00	0.00	0.00	0.00	124.99
0.35	0.00	0.00	0.00	0.00	129.30
0.35	0.00	0.00	0.00	0.00	133.61
0.00	0.64	0.00	0.00	0.00	137.93
0.00	0.64	0.00	0.00	0.00	142.24
0.00	0.64	0.00	0.00	0.00	146.55
0.00	0.64	0.00	0.00	0.00	150.87
0.00	0.64	0.00	0.00	0.00	155.18
0.00	0.00	0.43	0.00	0.00	159.49
0.00	0.00	0.43	0.00	0.00	163.81
0.00	0.00	0.43	0.00	0.00	168.12
0.00	0.00	0.43	0.00	0.00	172.44
0.00	0.00	0.43	0.00	0.00	176.75
0.00	0.00	0.00	0.62	0.00	181.06
0.00	0.00	0.00	0.62	0.00	185.38
0.00	0.00	0.00	0.62	0.00	189.69
0.00	0.00	0.00	0.62	0.00	194.00
0.00	0.00	0.00	0.62	0.00	198.32
0.00	0.00	0.00	0.00	0.45	202.63
0.00	0.00	0.00	0.00	0.45	206.94
0.00	0.00	0.00	0.00	0.45	211.26
0.00	0.00	0.00	0.00	0.45	215.57
0.00	0.00	0.00	0.00	0.45	219.88

The results of the multi-collinearity test are presented in Table 5.6.

Table 5.6 Multi-collinearity test

	Total cost	Cost underestimation	Budget conformity	Cost overrun	Financial exposition	Contingency cost
Total cost	1.00					
Cost underestimation	-0.46	1.00				
Budget conformity	-0.04	-0.23	1.00			
Cost overrun	-0.07	-0.23	-0.24	1.00		
Financial exposition	0.26	-0.23	-0.23	-0.24	1.00	
Contingency cost	0.30	-0.24	-0.24	-0.25	-0.24	1.00

The results indicate that cost underestimation, budget conformity and cost overrun have a negative correlation with the total cost whereas financial exposition and contingency cost have a positive correlation with the total cost. This indicates that the total cost calculated has a negative influence from cost underestimation, budget conformity and cost overrun and the actual total cost could be under-reported due to these factors. Because financial exposition and contingency cost have a positive influence on the total cost and due to these two factors, the actual total cost could be over-reported. While analysing Table 5.6 for inter-relationships among the cost risk factors, it can be inferred that the relationship between the predictors themselves seems to be low, which shows the absence of multi-collinearity and hence predictors are independent of each other. The key results of multiple regression analysis are presented in Table 5.7.

Table 5.7 Coefficients and p-value for each risk factor

Category	Coefficient	p-value
Intercept	107.11	5.0×10^{-3}
Cost underestimation	-97.11	0.19
Budget conformity	2.90	0.96
Cost overrun	-2.54	0.97
Financial exposition	77.98	0.31
Contingency cost	89.71	0.26

The results of regression analysis showed that for the given data set, the coefficient of determination (R square value) is 0.30 and the adjusted R square value is 0.23. The analysis showed a standard error of 55.28 and a significance F of 5.0x10-3. The high value of standard error and low value of adjusted R square are discussed in the VaR model input section of this paper.

Table 5.7 shows the coefficients and p-value of the data. The p-value here is the probability of an observed result, which has the assumption of the null hypothesis being true. This reveals that the null hypothesis (which states that all coefficients are zero) can be rejected based on its low p-value. In other words, a predictor with low p-value would be a meaningful addition to the current model, as changes in predictor values are associated with those of response variables. However, in case of large p-values, the changes in the values of the predictor are not associated with alterations in the values of the response variable. This indicates a condition of a statistically insignificant variable in the regression model. For the current work, a p-value and Significance F value, both less than 0.05, are used as criteria for a factor to be statistically significant and factors higher than these criteria are rejected systematically using the backward elimination method. In this method, variables with the highest p-value (statistically insignificant) are dropped and the regression analysis is run again. In the results above, since cost overrun has the highest p-value, it is a statistically insignificant variable; therefore, it is neglected and regression analysis is performed again. The regression performed after dropping the cost overrun showed that the p-values of risk factors cost underestimation, budget conformity, financial exposition and contingency cost are 0.035, 0.913, 0.082 and 0.054 respectively. The result shows that cost underestimation, financial exposition and contingency cost are statistically significant risk factors while budget conformity is a statistically insignificant risk factor and therefore does not pass the p-value test and can be neglected using the backward elimination method. The results of regression analysis performed by eliminating budget conformity show that the p-values of cost underestimation, financial exposition and contingency cost are 0.016, 0.058 and 0.035 respectively. This indicates that cost underestimation and contingency cost are statistically significant risk factors, while financial exposition is a statistically insignificant risk factor and can be eliminated from the analysis. The regression analysis performed after eliminating financial exposition shows that cost underestimation and contingency cost have p-values of 0.003 and 0.116 respectively. Since the p-value of the contingency cost is greater than 0.05, this risk factor is statistically insignificant and therefore can be neglected in the analysis. The regression analysis performed after eliminating the contingency cost shows that the p-value of cost underestimation is 8.84×10^{-4} and Significance F value is 8.48×10^{-4}, while its coefficient is -134.71. Since both the p-value and Significance F have values lower than the criteria set, cost underestimation qualifies to become a statistically significant risk factor in the analysis. The results show an intercept value of 127.67. With these results, the total cost model can be written as:

Total cost (estimated) = 127.67 – 134.71 x (cost underestimation)

This is interpreted to signify that for a one-dollar rise in cost underestimation, there is a decrease in total cost (estimated) by 134.71 dollars. Since the equation also includes the intercept, it can be interpreted that for a unit dollar of cost underestimation, the total cost (estimated) is -$7.04. This shows that total (estimated) cost is being calculated less by $7.04 for each unit dollar of cost underestimation and hence this value should be added to the total (estimated) cost to find the actual total cost. The actual total cost is defined as the total cost, which includes the impact of biodiesel cost related risk factors.

Actual total cost ($) = estimated total cost ($) + $7.04

The results of actual total cost for 5 years of biodiesel plant operations are shown in Table 5.8.

Table 5.8 Biodiesel actual total cost

Time (year)	Estimated total cost ($ million)	Actual total cost ($ million)
0	1.25	8.29
1	3.07	10.11
2	18.28	25.33
3	27.76	34.80
4	31.07	38.11
5	34.39	41.43

The cumulative probability profile developed as a result of Monte Carlo Simulation for year 2 is shown in Figure 5.5. The profile is showing VaR analysis for a 5% chance for year 2.

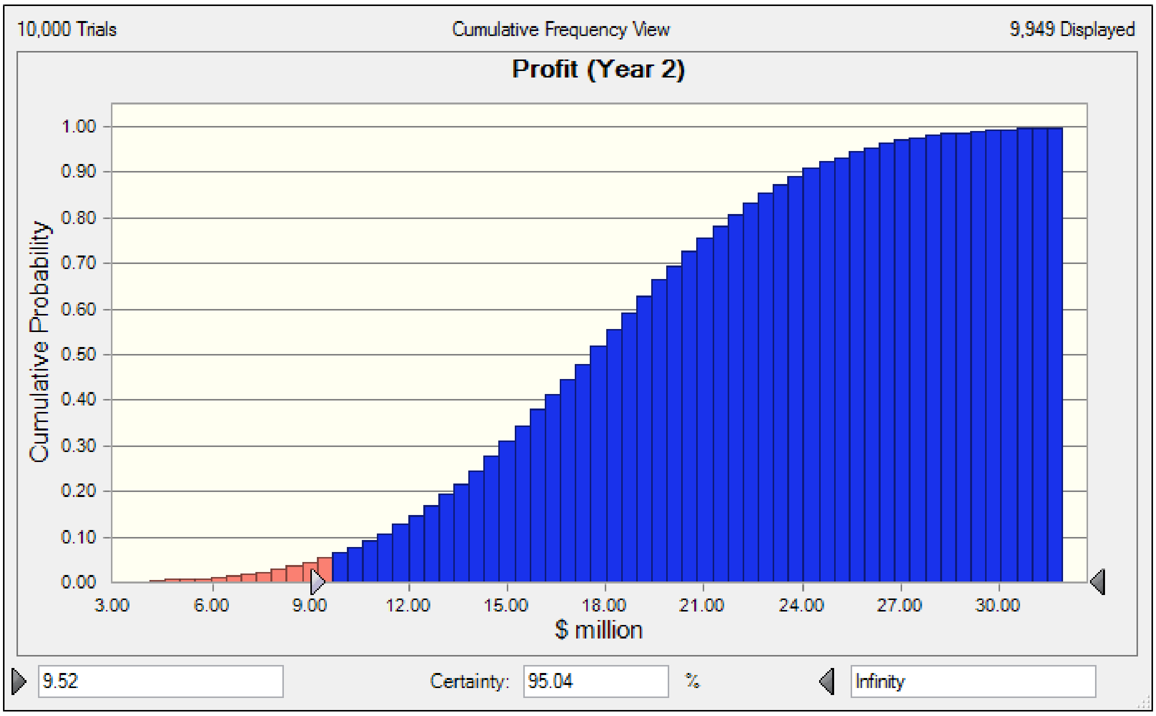


Figure 5.5 Cumulative probability profile for year 2

The results of VaR analysis for 1 VaR (1% chance), 5 VaR (5% chance) and 10 VaR (10% chance) for years 2, 3, 4 and 5 are shown in Table 5.9.

Table 5.9 1 VaR, 5 VaR and 10 VaR analyses

Time (Year)	**Total cost ($ million)**	**Revenue ($ million)**	**Profit ($ million)**	**1 VaR ($ million)**	**5 VaR ($ million)**	**10 VaR ($ million)**
0	8.29	0	0	0	0	0
1	10.11	0	0	0	0	0
2	25.33	43.05	17.72	6.26	9.52	11.34
3	34.81	94.71	59.90	36.50	43.03	47.01
4	38.12	104.18	66.06	40.02	47.49	51.40

5	41.44	114.60	73.16	44.16	53.38	57.52

The results show that 1 VaR for year 2 is $6.26 million. The interpretation of this result is that there is a 99% chance that profit will not fall below $6.26 million over the period of 2 years of plant operations. In other words, there is a 1% chance that profit would be reduced to $6.26 million or below in year 2, which is the monetary value-at-risk. Since the cumulative probability profile of profit was generated through 10,000 trials in Monte Carlo Simulation, the results can also be interpreted in terms of number of trials. In terms of number of trials, out of 10,000 trials, for 1 VaR, there are only 100 (1% of 10,000) chances that the profit would be reduced to $6.26 million or below, which is a much less possibility considering the total number of trials, though a high dollar value (in million dollars) is at risk. In other words, there are 9,900 (99% of 10,000) chances that profits would not go below $6.26 million in year 2 of operation, which, considering the number of the total trials, is a high possibility. In year 3, 1 VaR is $36.50 million. This shows that there is a 1% chance that in year 3, profit will be reduced to $36.50 or below. Conversely, there is a 99% chance that the maximum profit reduced in year 3 will be $36.50 million. In years 4 and 5, 1 VaR is $40.02 and $44.16 million respectively. This shows that in years 4 and 5 respectively there is a 1% chance that profit will be reduced to $40.02 million or less in year 4 and $44.16 million or less in year 5. The VaR (1 VaR, 5 VaR or 10 VaR) increases over the period since the profit is increasing annually, as is the risk associated with it. The results of 5 VaR and 10 VaR show that in year 2, 5 VaR is $9.52 million and 10 VaR is $11.34 million. This indicates that there is a 5% chance that profit will fall to $9.52 million or below in year 2 and a 10% chance that profit will fall to % $11.34 million or below in the same year. This shows that the lower the degree of assurance, the higher is the VaR profits. Table 5.9 shows that in years 0 and 1 there is no VaR. This is because, according to the plant's start-up schedule, there is no biodiesel production in years 0 and 1 and since no revenue or profit is earned in this period, there will be no risk associated with profit. Since the VaR analysis is based on the actual total cost, which includes the impact of cost related risk factors, the analysis represents a true picture of risks on returns.

The relation between the profit certainty level and payback period is studied below. Figure 5.6 represents the impact of the VaR study on the payback period.

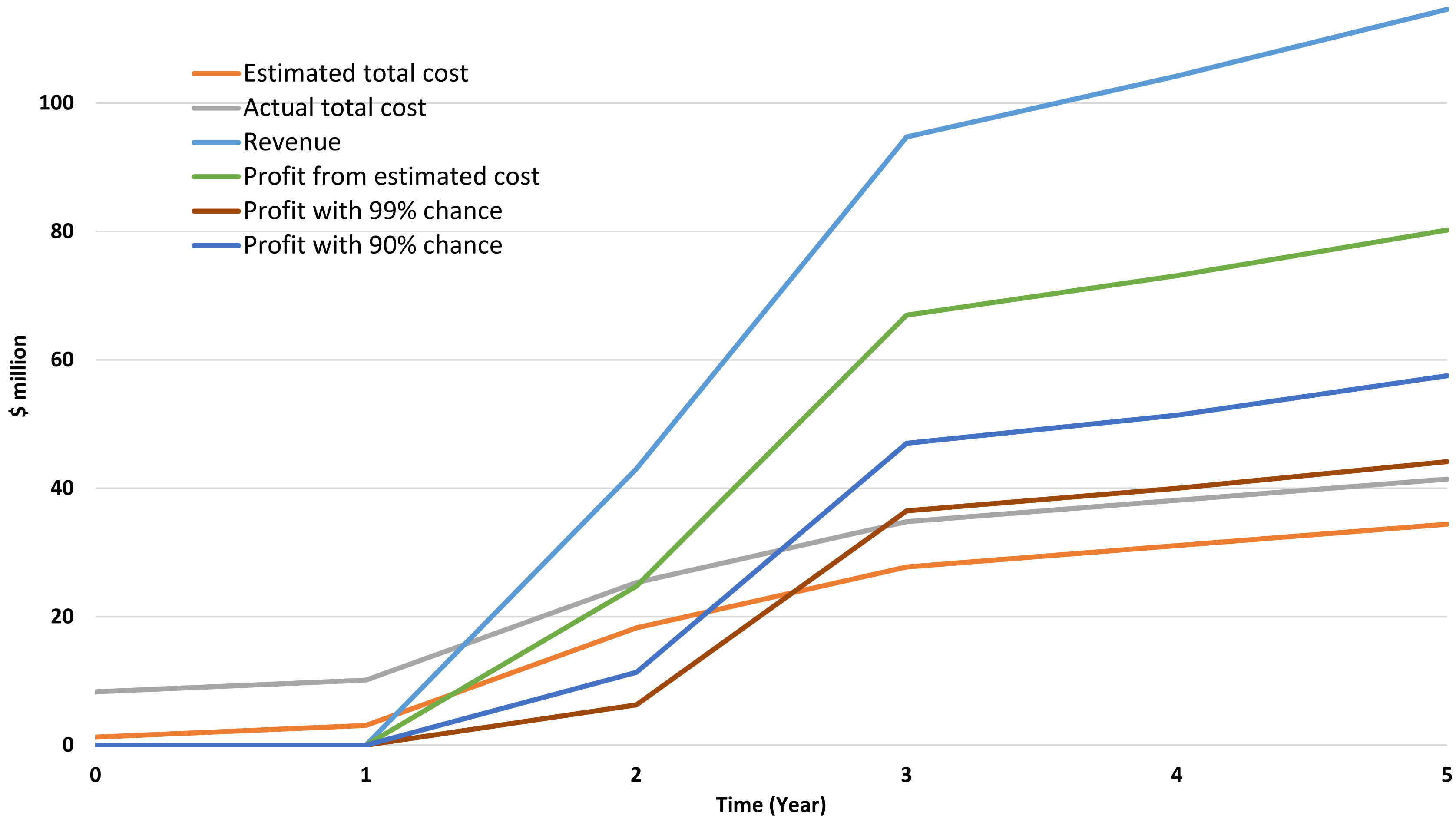


Figure 5.6 Profit certainty level and Payback Period

The graph shows the relationship among revenue earned, actual total cost spent, estimated total cost and the profit earned from biodiesel production over the period of five years. Based on VaR results, the profit earned with a 99% chance is analysed for the payback period. The results show that the profit calculated from estimated total cost has a payback period of 1.25 years or 15 months after the plant starts to produce and sell biodiesel. However, when the cost related risk factors are included in the study, the payback period is affected. Figure 5.6 shows that the payback period for the actual cost is 2.9 years ≈ 3 years (36 months). This shows that the inclusion of cost related risk factors has increased the payback period by 21 months, which represents the true payback period, since cost related risk factors do influence cost estimation. This highlights the importance of introducing cost related risk factors in calculating the total cost of production. Figure 5.6 shows that the profit earned with a 90% chance has a payback period of 2.5 years, while for a 99% chance, it is 3 years. This implies that a higher degree of confidence in earning profits is associated with a delay in the return period. These results show that with the need of a higher confidence level in profit making, a biodiesel investor will have to consider a longer time to receive returns. The results also indicate the importance of including biodiesel cost related risk factors in the techno-economical study of a biodiesel production plant using VaR analysis. The impact of cost risk factors on profit is shown in Figure 5.7.

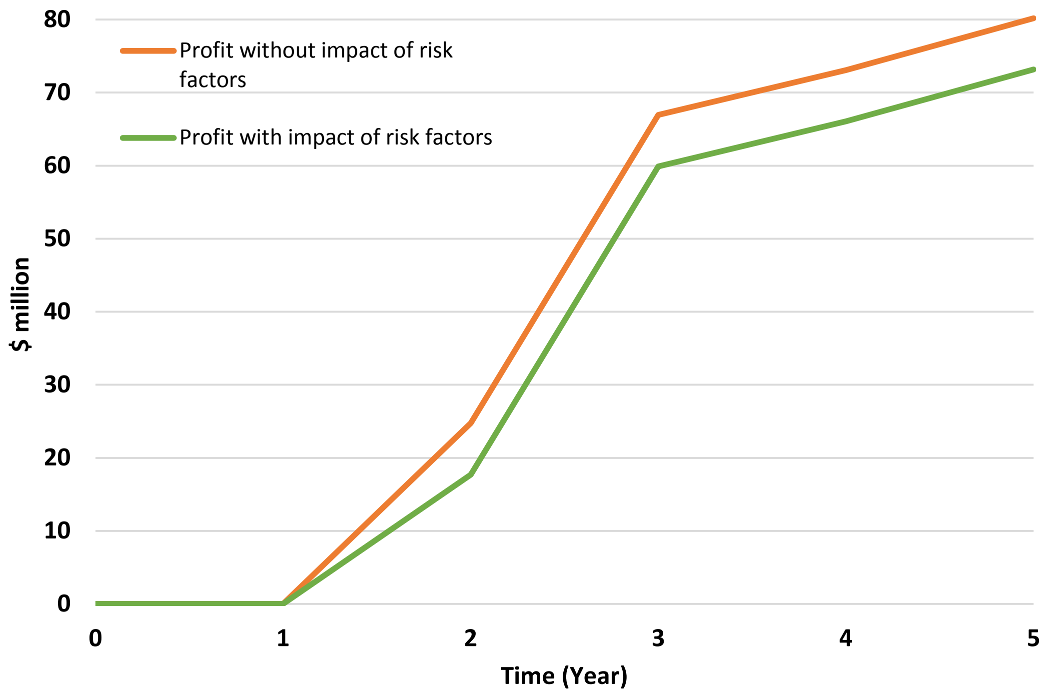


Figure 5.7 Impact of cost risk factors on profit

Figure 5.7 shows the profit profiles with and without considering the risk factors in the biodiesel process economical study. This shows that although biodiesel profit may seem to be high over the period of five years and to increase thereafter, when biodiesel cost related risk factors were introduced into the study, they made a huge impact on biodiesel profit and decreased the profit each year. The expected profit earned without considering the impact of cost risk factors in year 5 is $80.20 million. When profit earned by incorporating the impact of cost related risk factors was added to the total cost, the profit dropped to $73.16 million. Over the period of five years, the actual profit could be $7.04 million ($80.20 million - $73.16 million) less than expected. This result is because risk factors have increased the total cost of biodiesel production while it has the same revenue. In this analysis, a huge quantity of biodiesel production is analysed with an aim to produce more profit along with more quantity; however, the results indicate that with a large biodiesel plant capacity, careful consideration of the cost related risk factors could guarantee a higher profit selling biodiesel.

5.5 Discussion on VaR model inputs

In this study, the VaR model developed was analysed based on an expert's inputs and the inferred results were based on that. The expert's inputs were used for two steps. Firstly, a structural self-interaction matrix was developed with which an expert was then to provide a pairwise comparison of risk factors. This was qualitative input data from the expert. In doing so, the expert was supposed to provide 20 qualitative inputs (as shown in Table 5.2) to develop a structural self-interaction matrix. Secondly, conditional probabilities tables were developed and marginal probabilities were allocated for Bayesian Network analysis. This was quantitative input data from the same expert. The expert was supposed to provide 13 quantitative inputs (as shown in Figure 5.4). These were 4 inputs for budget conformity, 4 inputs for contingency cost, 2 inputs for cost underestimation, 2 inputs for cost overrun and one input for the probability of a financial exposition cost risk factor. In total, there was a need to take 33 inputs from an expert to analyse the VaR model developed. In the current study, one expert input was taken to demonstrate the VaR methodology developed. It is believed that given the right input data, the analysis would be different and this would definitely reduce the standard error and increase adjusted R square values in multiple regression analysis. It is also recommended to take inputs from more than one expert and use their average value for each input point. The experts could include biodiesel investors, biodiesel researchers, shareholders, business partners, management and biodiesel industry financial stakeholders. The inputs could be taken through direct interviews in which stakeholders would have an opportunity to ask questions. The opinions of experts integrated with the simulations and methodology proposed in this analysis would help biodiesel risk managers to make risk management decisions, which would influence overall biodiesel plant production. This would help in critical investment decision-making while considering different financial risk exposures in biodiesel financial risk management.

5.6 Conclusion

A novel process economics methodology comprised of value at risk (VaR) is proposed here. Its application is demonstrated using a biodiesel production system. The VaR concept was used to demonstrate the economic risk of process operations. In this analysis, VaR was defined as the successful use of the biodiesel. The study was performed for a biodiesel plant having a production capacity of 45,000 tonnes of biodiesel per annum. Different cost related risk factors such as cost underestimation, budget conformity, financial exposition, cost overrun and contingency cost influence VaR. The study shows that each individual risk factor in a network influences the total cost of biodiesel production and the objectives of VaR.

The qualitative results of interpretive structural modelling (ISM) are shown in a network of influence, where contingency cost is influencing budget conformity while it is being influenced by cost overrun and financial exposition. Budget conformity is being influenced by cost overrun and contingency cost, while it is not influencing any other risk factor in the network. Financial exposition is influencing cost underestimation and contingency cost while cost underestimation is influencing cost overrun. The ISM network is transformed into a Bayesian network to do a quantitative analysis. The results of quantitative analysis indicate that cost underestimation has the highest influence on a risk network, while budget conformity has the least impact. The results of multiple regression analysis revealed that cost underestimation is the only statistically significant risk factor and that it affects the total cost estimated.

The VaR analysis reveals that 1 VaR is $6.26 million for year 2 which means that there is a 99% chance that biodiesel profit will not to fall below $6.26 million over the period of 2 years of plant operations. The analysis also showed that 5 VaR is $53.38 million for year 5 which shows that over the period of five years, there is a 5% chance that profit will fall to $53.38 million or below. This helps biodiesel investors to forecast their losses over 5 years of plant operations based on a given probability level. The results of the VaR model also show that due to integration of cost related risk factors; the project payback period is increased by 21 months. This suggests controlling and mitigating cost related risk factors for a successful biodiesel business. The forecasted risk can help investors and management to better plan, allocate resources, energy, material, work force and finances.

This work requires further testing on different process facilities. This work could be improved by considering accidental events or losses within the tail end of distribution, consideration of a conditional VaR model for process facilities, and inclusion of other risk factors such as market risk factors.

5.7 References

Atabani, A. E., A. S. Silitonga, H. C. Ong, T. M. I. Mahlia, H. H. Masjuki, I. A. Badruddin and H. Fayaz (2013). "Non-edible vegetable oils: A critical evaluation of oil extraction, fatty acid compositions, biodiesel production, characteristics, engine performance and emissions production." Renewable and Sustainable Energy Reviews 18: 211-245.

Balat, M. and H. Balat (2010). "Progress in biodiesel processing." Applied Energy 87(6): 1815-1835.

Bandara, R. and D. Dassanayake (2006). "A quantitative analysis on factors affecting profitability of small scale broiler production." The Journal of Agricultural Sciences 2(3): 45-50.

Banković-Ilić, I. B., O. S. Stamenković and V. B. Veljković (2012). "Biodiesel production from non-edible plant oils." Renewable and Sustainable Energy Reviews 16(6): 3621-3647.

Beneda, N. (2005). "Managing an asset management firm's risk portfolio." Journal of Asset Management 5(5): 327-337.

Bohdalová, M. (2007). "A comparison of value-at-risk methods for measurement of the financial risk." Faculty of Management, Comenius University, Bratislava, Slovakia.[Online], E-learning working paper,[Online] Retrieved 10 June 2016, from http://www.g-casa.com/PDF/Bohdalova.pdf.

Cakir, H. M. and U. Uyar (2013). "Portfolio Risk Management with Value at Risk: A Monte-Carlo Simulation on ISE-100." International Research Journal of Finance and Economics(109): 118.

Chatterjee, S. and A. S. Hadi (2015). Regression analysis by example, John Wiley & Sons.

Chen, H., D. Zhou, G. Luo, S. Zhang and J. Chen (2015). "Macroalgae for biofuels production: Progress and perspectives." Renewable and Sustainable Energy Reviews 47: 427-437.

Cheung, Y. H. and R. J. Powell (2012). "Anybody can do value at risk: a nonparametric teaching study." Australasian Accounting, Business and Finance Journal 6(1): 111-123.

Cheung, Y. H. and R. J. Powell (2013). "Anybody can do value at risk: a teaching study using parametric computation and Monte Carlo simulation." Australasian Accounting, Business and Finance Journal 6(5): 101-118.

Colin, J., D. Estampe, H.-C. Pfohl, P. Gallus and D. Thomas (2011). "Interpretive structural modeling of supply chain risks." International Journal of physical distribution & logistics management 41(9): 839-859.

Culp, C. L. (2002). The Risk Management Process: Business Strategy and Tactics, John Wiley & Sons.

Eguchi, S., S. Kagawa and S. Okamoto (2015). "Environmental and economic performance of a biodiesel plant using waste cooking oil." Journal of Cleaner Production 101: 245-250.

Farooq, A., M. Ishaq, N. Shah, A. Hassan and K. Nabi (2013). "Economies of scale in broiler farming in Khyber Pakhtunkhwa." Sarhad Journal of Agriculture 29: 119-126.

Fasahati, P., H. C. Woo and J. J. Liu (2015). "Industrial-scale bioethanol production from brown algae: Effects of pretreatment processes on plant economics." Applied Energy 139: 175-187.

Formighieri, C. (2015). Biodiesel from Microalgae. Solar-to-fuel conversion in algae and cyanobacteria, Springer: 19-26.

Gerpen, J. V. (2005). "Biodiesel processing and production." Fuel Processing Technology 86(10): 1097-1107.

J., L. T. and P. N. D. (2000). "Value at Risk." Financial Analysts Journal 56(2): 47-67.

Jorion, P. (2006). Value at Risk: The New Benchmark for Managing Financial Risk, McGraw-Hill Education.

Kinney, A. J. and T. E. Clemente (2005). "Modifying soybean oil for enhanced performance in biodiesel blends." Fuel Processing Technology 86(10): 1137-1147.

Kraha, A., H. Turner, K. Nimon, L. R. Zientek and R. K. Henson (2012). "Tools to support interpreting multiple regression in the face of multicollinearity." Sweating the Small Stuff: Does data cleaning and testing of assumptions really matter in the 21st century?: 76.

Lozowski, D. (2016). "The Chemical Engineering Plant Cost Index." Retrieved July 10, 2016, from http://www.chemengonline.com/pci-home.

Nimon, K. F. and F. L. Oswald (2013). "Understanding the results of multiple linear regression beyond standardized regression coefficients." Organizational Research Methods 16(4): 650-674.

Ofori-Boateng, C. and K. T. Lee (2011). Feasibility of jatropha oil for biodiesel: economic analysis. World Renewable Energy Congress-Sweden; 8-13 May;

2011; Linköping; Sweden, Linköping University Electronic Press Retrieved 22 June 2016, from http://www.ep.liu.se/ecp/057/vol1/062/ecp57vol1_062.pdf.

Olson, D. L. and D. Wu (2010). Value at Risk. Enterprise Risk Management Models. Berlin, Heidelberg, Springer Berlin Heidelberg: 131-141.

Renda, R., E. Gigli, A. Cappelli, S. Simoni, E. Guerriero and F. Romagnoli (2016). "Economic Feasibility Study of a Small-scale Biogas Plant Using a Two-stage Process and a Fixed Bio-film Reactor for a Cost-efficient Production." Energy Procedia 95: 385-392.

Sadeghi, M. and S. Shavvalpour (2006). "Energy risk management and value at risk modeling." Energy policy 34(18): 3367-3373.

Sajid, Z., F. Khan and Y. Zhang (2016a). "Integration of Interpretive Structural Modelling with Bayesian Network for Biodiesel Performance Analysis." Under review.

Sajid, Z., F. Khan and Y. Zhang (2016b). "Process simulation and life cycle analysis of biodiesel production." Renewable Energy 85: 945-952.

Sajid, Z., Y. Zhang and F. Khan (2016). "Process design and probabilistic economic risk analysis of bio-diesel production." Sustainable Production and Consumption 5: 1-15.

Sambusiti, C., M. Bellucci, A. Zabaniotou, L. Beneduce and F. Monlau (2015). "Algae as promising feedstocks for fermentative biohydrogen production according to a biorefinery approach: A comprehensive review." Renewable and Sustainable Energy Reviews 44: 20-36.

Shah, S. (2005). "Biofuels seeks cash after cost overruns." Business News UK Retrieved 9 May 2016, 2016, from http://www.independent.co.uk/news/business/news/biofuels-seeks-cash-after-cost-overruns-5886.html.

Ullah, K., M. Ahmad, Sofia, V. K. Sharma, P. Lu, A. Harvey, M. Zafar and S. Sultana (2015). "Assessing the potential of algal biomass opportunities for bioenergy industry: A review." Fuel 143: 414-423.

Vassilev, S. V. and C. G. Vassileva (2016). "Composition, properties and challenges of algae biomass for biofuel application: An overview." Fuel 181: 1-33.

Venkatesh, V. G., S. Rathi and S. Patwa (2015). "Analysis on supply chain risks in Indian apparel retail chains and proposal of risk prioritization model using Interpretive structural modeling." Journal of Retailing and Consumer Services 26: 153-167.

Wu, L., T. Wei, Z. Lin, Y. Zou, Z. Tong and J. Sun (2016). "Bentonite-enhanced biodiesel production by NaOH-catalyzed transesterification: Process optimization and kinetics and thermodynamic analysis." Fuel 182: 920-927.

Zou, K. H., K. Tuncali and S. G. Silverman (2003). "Correlation and simple linear regression 1." Radiology 227(3): 617-628.

Chapter 6

6 Process simulation and life cycle analysis of biodiesel production

Authorship and contributorship

This work has been published by Sajid, Z., Khan, F., & Zhang, Y. (2016). "Process simulation and life cycle analysis of biodiesel production". *Renewable Energy*, 85, 945-952.

This article can be accessed through the following link:

http://www.sciencedirect.com/science/article/pii/S0960148115301415

The co-authors, Dr. Yan Zhang and Zaman Sajid formulated the research problem. The first author, Zaman Sajid structured the approach, designed and conducted the analysis, executed the life cycle study and drafted the manuscript. The co-authors, Drs. Faisal Khan & Yan Zhang, critically reviewed the developed approach, and provided valuable suggestions to improve both the approach and the presentation of the results in the manuscript. The first author, Zaman Sajid, has implemented feedback from the co-authors and peer reviewers.

Abstract

Biodiesel is a renewable and sustainable biofuel. There are various production processes to produce biodiesel from different kinds of raw materials. In this study, the environmental impacts of biodiesel production from non-edible Jatropha oil and waste cooking oil (WCO) were investigated and compared using systematic life cycle assessment. The results show that crops growing and cultivation of non-edible Jatropha oil lead to higher environmental impacts compared to WCO process. However, biodiesel production process from Jatropha oil has better performance because the WCO process needs to consume variety of chemicals and requires a large amount of energy for the pre-treatment of raw WCO and further chemical conversion to biodiesel. Results also indicate that the collection mechanism of WCO has significant contributions towards environmental impacts. In general, biodiesel production from Jatropha oil shows higher impacts for damage categories of climate change, human health and ecosystem quality whereas biodiesel production from WCO has more severe environmental impacts for resource category. The total environmental impact is 74% less in case of using WCO as raw material compared to non-edible Jatropha oil.

6.1 Introduction

In 2012, United States has been the major consumer of crude oil in the world (Energy 2014). This consumption is linked with increased demand of crude oil as transport fuel and is continuously depleting natural resources of fossil fuel. Besides these facts, the consumption of conventional crude oil is contributing to severe environmental impacts. One of those impacts is the global warming (Omer 2008a). As an alternate fuel to conventional crude oil, biodiesel has the potential to reduce the dependency on natural resources and greenhouse gas emissions (Omer 2008b).

The production of biofuel from biomass depends on two major factors. First, the availability of raw material for biofuel and second, the process adopted to produce biofuel. Abbaszaadeh et al. (2012) summarized different biodiesel production technologies. The most widely used process to produce biodiesel is the trans-esterification, a chemical reaction between biomass feedstock and an alcohol in the presence of a catalyst. The reaction bi-products are biodiesel, chemically known as ethyl or methyl esters, and glycerol. The biomass feedstock could be vegetable oil or animal fat. In edible oils, typically, soybean oil, sunflower oil, rapeseed oil, and palm oil are used as raw materials. Since these raw materials are also used as food, their abundant use to produce biofuel (energy) can lead to shortage of food.

In order to avoid this conflict between energy and food demand, in recent years, the research has been shifted to produce biodiesel from non-edible resources (Achten, Verchot et al. 2008; Lu, Liu et al. 2009; Cynthia and Lee 2011; Raja, Smart et al. 2011; Atabani, Silitonga et al. 2013). Though the use of non-edible resources as biomass feedstock eliminates the debate of food and energy scarcity, the non-edible biomass feedstock still requires the use of land to grow crops. But the requirement of land is much less demanding as compared to those for edible biomass feedstocks preparations (Banković-Ilić, Stamenković et al. 2012). The non-edible biomass feedstocks include mainly the oils from non-edible vegetables, such as *Jatropha curcas* (Jatropha) (Sahoo and Das 2009; Huerga, Zanuttini et al. 2014), *Linum usitatissimum* (Linseed) (Borugadda and Goud 2012), *Simmondsia chinesnsis* (Jojoba) (Shah, Ali et al. 2014), *Hevea brasiliensis* (rubber seed) (Bharathiraja, Chakravarthy et al. 2014), *Azadirachta indica* (Neem) (Ali, Mashud et al. 2013), Cotton seed (Royon, Daz et al. 2007), *Calophyllum inophyllum* (Polanga) (Sahoo and Das 2009), *Nicotianna tabacum* (tobacco) (Usta, Aydogan et al. 2011), *Pongamia pinnata* (karanja) (Dhar and Agarwal 2014) and *Maduca indica* (mahua) (Puhan, Vedaraman et al. 2005).

Studies have been carried out to scrutinize the physicochemical properties of biodiesel produced from these non-edible biomass feedstocks (Atabani, Silitonga et al. 2013; Ashraful, Masjuki et al. 2014). Other than non-edible vegetable oils, research is underway to use waste cooking oil (WCO) as potential biomass feedstock to produce biodiesel (Naima and Liazid 2013; Gopal, Pal et al. 2014). The availability of WCO comes from different resources, including commercial, industrial, and domestic sources.

The advantages of using WCO to produce biodiesel are threefold. First, it can significantly decrease the amount of farmland, which is necessary for biodiesel producing corps. Second, the usage of WCO also helps to reduce biodiesel production costs (Zhang, Dube et al. 2003; Haas, McAloon et al. 2006; Kulkarni and Dalai 2006; Marchetti, Miguel et al. 2008). Third, the waste management of WCO is a problematic step and its use as biofuel raw material reduces the cost of waste product removal and treatment. In the light of above facts, research has recently been focused on the use of WCO as raw material to produce biodiesel (Phan and Phan 2008; Hasibuan, Ma'ruf et al. 2009; Refaat 2010; M and D 2014). However, there are also few disadvantages associated with the use of WCO as biodiesel raw material, during the frying of cooking oil, free fatty acid and other products namely polymerized triglycerides are formed in oil. These products effect the trans-esterification reaction for biodiesel production (Kulkarni and Dalai 2006). The collection and supply chain mechanism of WCO in some countries has not been sufficiently develop (Ramos, Gomes et al. 2013; Cho, Kim et al. 2015) and research is being conducted to develop an effective WCO collection mechanism (Singhabhandhu and Tezuka 2010).

From the production point of view, either of these raw materials can be used to produce biofuel by trans-esterification. However, from environmental perspective, the choice between these raw materials is not straight forward as the use of both raw materials has their respective advantages and disadvantages. The trans-esterification of non-edible oil seems to be simple and the raw material requires no special treatment, which helps to reduce the chemical consumptions in the production process. However, the preparation of non-edible biomass requires crop cultivation, which consumes fertilizers, chemicals, conventional fuels, water, pesticides, and energy – thus generating high environmental impacts. On the other hand, a pre-treatment of WCO is essential before it is converted to biodiesel through trans-esterification. This pre-treatment requires different kinds of chemicals and have different energy requirements, which also engender significant environmental impacts. Although biodiesel production from WCO does not need to use fertilizers, land and water for biomass culture, a collection system has to be developed to collect the WCO from different resources. Clearly, no apparent solution is available to evaluate which raw material provides less environmental damages unless a complete systematic study is conducted. One of the tools employed for quantitative assessment of the environmental impacts (greenhouse gas emissions (GHG), resource consumption and depletion, and human health impacts, etc.) of biodiesel production is the life cycle assessment (LCA). LCA helps to evaluate the environmental impacts of a product over its entire life – from the preparation of raw material, through the manufacturing of product and its use, reuse and disposal at the end of its useful life (Kiwjaroun, Tubtimdee et al. 2009).

In recent years, a number of studeis have been undertaken to estimate the environemtal impacts of biodiesel production from various biomass feedstock. Farrell & Cavanagh (2014) studied the environmental impacts of biodiesel from waste vegetable oil and fresh vegetable oil and made a comparison of the results with those of petroleum diesel. Kaewcharoensombat et al (2011) studied LCA of biodiesel production from Jatropha oil using two different catalysts, i.e., sodium hydroxide and potassium hydroxide. They studied eleven environmental categories except global warming, which is an important environmental impact category. Morais et al (2010) performed simulation and an LCA of three process design alternatives for biodiesel production using waste cooking oil as raw material. Their simulation for alkali-catalysed process with free fatty acid (FFA) pre-treatment did not include any treatment of unconverted oil stream neither it was considered as a waste in their LCA studies.

Previous LCA studies of biodiesel focus on few environmental impacts and do not present the complete picture of environmental damages. As shown in the literature review, some of LCA studies, even, do not include complete production process in their analysis. The production stage of biodiesel has high requirements of material and energy and emits high wastes, therefore any waste or stream in production stage cannot be neglected without proper justification. Neglecting such streams might have huge environmental impacts, which could mislead the results of LCA. Moreover, previous studies do not provide an LCA on a comparative base. A unique system boundary and functional unit is required to compare two cases, as the LCA studies are highly dependent on these two factors.

This paper aims to study biodiesel produced from two different raw materials: the Jatropha oil and WCO using alkali-catalysed trans-esterification method. The LCA was performed on the preparation of respective raw materials, their production, industrial conversion of raw materials into biodiesel and biodiesel end use. Moreover, in case of Jatropha oil, the environmental damage due to crops growing, their harvesting, raw material transportation and seed-oil extraction was included. The environmental impacts of biodiesel production from WCO was also studied using its supply chain, collection technologies, the energy required in pre-treatment of WCO and quality of biomass. The production environmental load from each case was estimated by using a process simulator, Aspen HYSYS v7.3, for assessing the material and energy requirements. The results of the process simulation were used as input for LCA study. A detailed life cycle assessment on an equal comparison bases was also carried out.

6.2 Methodology

6.2.1 Process simulation

The production of biodiesel from biomass feedstock is a well-understood process. In the current study, alkali-catalysed trans-esterification process is studied to produce biodiesel. This process requires low reaction temperatures (66^{o}C) and low-pressure (20psi). Moreover, the reaction completes in a short time while provides high conversion factor (95%). The catalyst used in the current study is sodium hydroxide. In order to study the LCA of biodiesel production from Jatropha oil and WCO, the material and energy requirements, based on process flow sheeting, were required. In earlier publication, a biodiesel plant producing 45,000 t/yr. biodiesel was simulated in HYSYS (Sajid, Zhang et al. 2014). The plant utilises Jatropha oil as raw material to produce biodiesel. The results of material and energy balances were referred in this paper. In case of WCO, a biodiesel plant using WCO as raw material was simulated in HYSYS for the same production rate. Due to ease of availability, WCO provide a viable alternative to conventional diesel. The production of biodiesel from WCO is an energy efficient process (Mohammadshirazi, Akram et al. 2014). WCO collected from different resources contains approximately 6% free fatty acids. Such high free fatty acid contents make the raw WCO difficult to be directly reacted with methanol, in the presence of sodium hydroxide to produce biodiesel. Hence, a pre-treatment of raw WCO is prerequisite. The steps for pre-treatment of raw WCO and chemical conversion of WCO to biodiesel (alkyl ester) are as follows,

1) Filtration – removes any suspended solids in raw WCO
2) Reaction of methanol, sulphuric acid (5%) and filtered WCO – it produces methyl esters and stream contains sulphuric acid.

3) Glycerol washing, the stream from step two is washed with glycerol – it removes sulphuric acid in the stream and WCO produced has 0.3% free fatty acid contents. WCO is reacted with methanol in the presence of sodium hydroxide to produce biodiesel (Sajid, Zhang et al. 2014).
4) Bottom stream of glycerol washer is distilled to recover methanol – methanol is obtained at the top of distillation column, which is recycled into the system, and bottom stream contains glycerol and sulphuric acid.
5) Distilled bottom stream is reacted with calcium oxide followed by the gravity separator – the step converted sulphuric acid into calcium sulphate.
6) An evaporator is used to separate methanol and glycerol – glycerol is recycled into the process.

Figure 6.1 illustrates the process flow diagram of a biodiesel production plant, which utilizes WCO as feedstock. Aspen HYSYS was employed to simulate this biodiesel plant with a production capacity of 45,000 t/yr. The steps to perform the simulation included, defining the chemical components, selection of appropriate thermodynamic model and the selection of the stream conditions (mass or volumetric flow rate, temperature, pressure etc.). The library of HYSYS contained information regarding the physical properties of all components except WCO and its respective biodiesel. These components were defined in HYSYS as hypothetical components and the simulator estimated their properties.

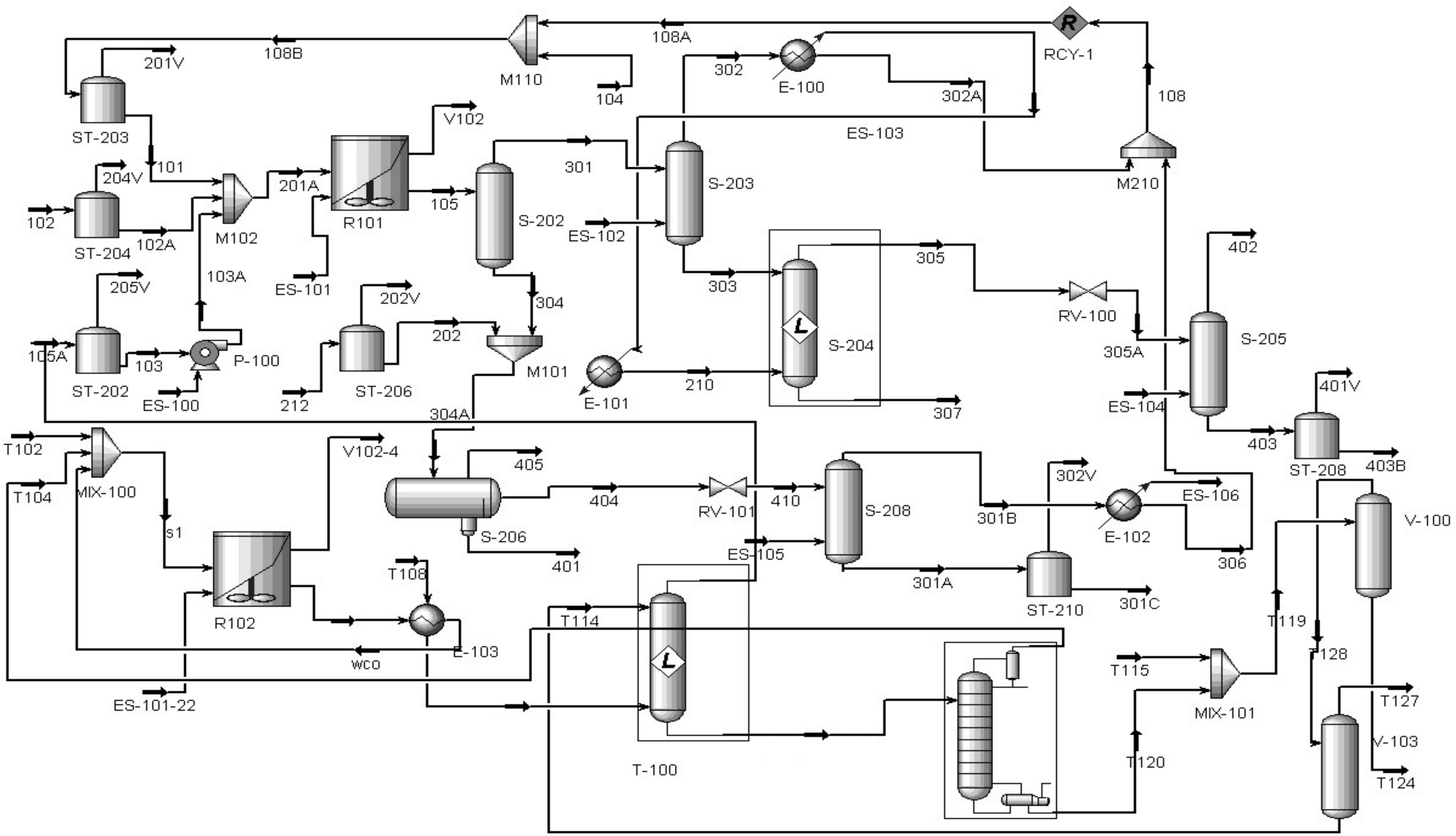


Figure 6.1 Alkali-catalysed process to produce biodiesel from WCO and its pre-treatment – a simulation in HYSYS

6.2.2 Life cycle analysis

In this study, LCA methodology was used as a tool to compare the environmental impacts of using both biomasses feed stocks for biodiesel production. LCA is a very helpful tool in addressing the linkage between biofuel systems and their environmental performances. This study was conducted according to framework defined by International Organization for Standardization (ISO) 14044:2006 standard. The requirements of which include goal and scope definition of LCA, life cycle inventory (LCI) analysis, life cycle impact assessment (LCIA) and data interpretation.

6.2.2.1 Goal and scope of the LCA

The goal of this LCA study includes the quantification and comparison of total environmental impacts to produce biodiesel from Jatropha oil and WCO. The study also analyses the flows of material and energy streams to produce biodiesel from both raw materials. The key factors, which affect the WCO biodiesel process, were also discussed in much detail.

6.2.2.2 Functional unit and system boundary

The functional unit for this study is the production of 1 ton of biodiesel using Jatropha oil and WCO. The comparison on equal mass bases accounts for different material and energy requirements to produce unit mass of biodiesel from different raw materials. In order to standardize the transportation costs, it was assumed that both feedstock were set up at the same location in the United States. Figure 6.2 shows the system boundary for LCA studies used in this work. The system boundary clearly defines all resources, chemicals, energy requirements, materials demands, pollution emissions, feedstock requirements, biomass and transportations of different materials, exhaust gases related to each process and energy outputs of the respective processes. The study includes a cradle to gate analysis assuming that the combustion of biodiesel, biodiesel produced by either of biomass feedstock, has same environmental impacts, and could be neglected while making a comparison. This assumption is based on fact that the combustion of biodiesel produced by either raw material has the same combustion properties and has the similar energy emissions, irrespective of biomass feedstock used to produce that biodiesel (Hou, Zhang et al. 2011).

More specifically, the system boundary for biodiesel production from Jatropha oil includes cultivation and harvesting of Jatropha crops, transportation and extraction of Jatropha seeds as well as chemical conversion of Jatropha oil to biodiesel by alkali-catalysed trans-esterification reaction. Whereas, the environmental damage arising from the biodiesel production from WCO was also examined by three phases. First – energy requirements in WCO supply chain and the collection mechanism to collect raw WCO from different resources at a single site. Second – the environmental impacts due to the transportation of this raw WCO to the chemical plant site for chemical conversion. Third – pre-treatment of raw WCO and the alkali-catalysed trans-esterification of treated WCO to produce biodiesel. Since the collection of WCO from different resources consumes much of fuel in transportation and the distances varies from location to location. Therefore, it is assumed that a higher distance is travelled to collect WCO as compared to the collection of Jatropha oil (Frischknecht, Jungbluth et al. 2007). Any kind of transportation is assumed by road using lorry. The capacity sizes of various Lorries chosen are discussed in next sections. The end-use of biodiesel is the combustion in a diesel vehicle and the combustion gases are obtained with no soot formation.

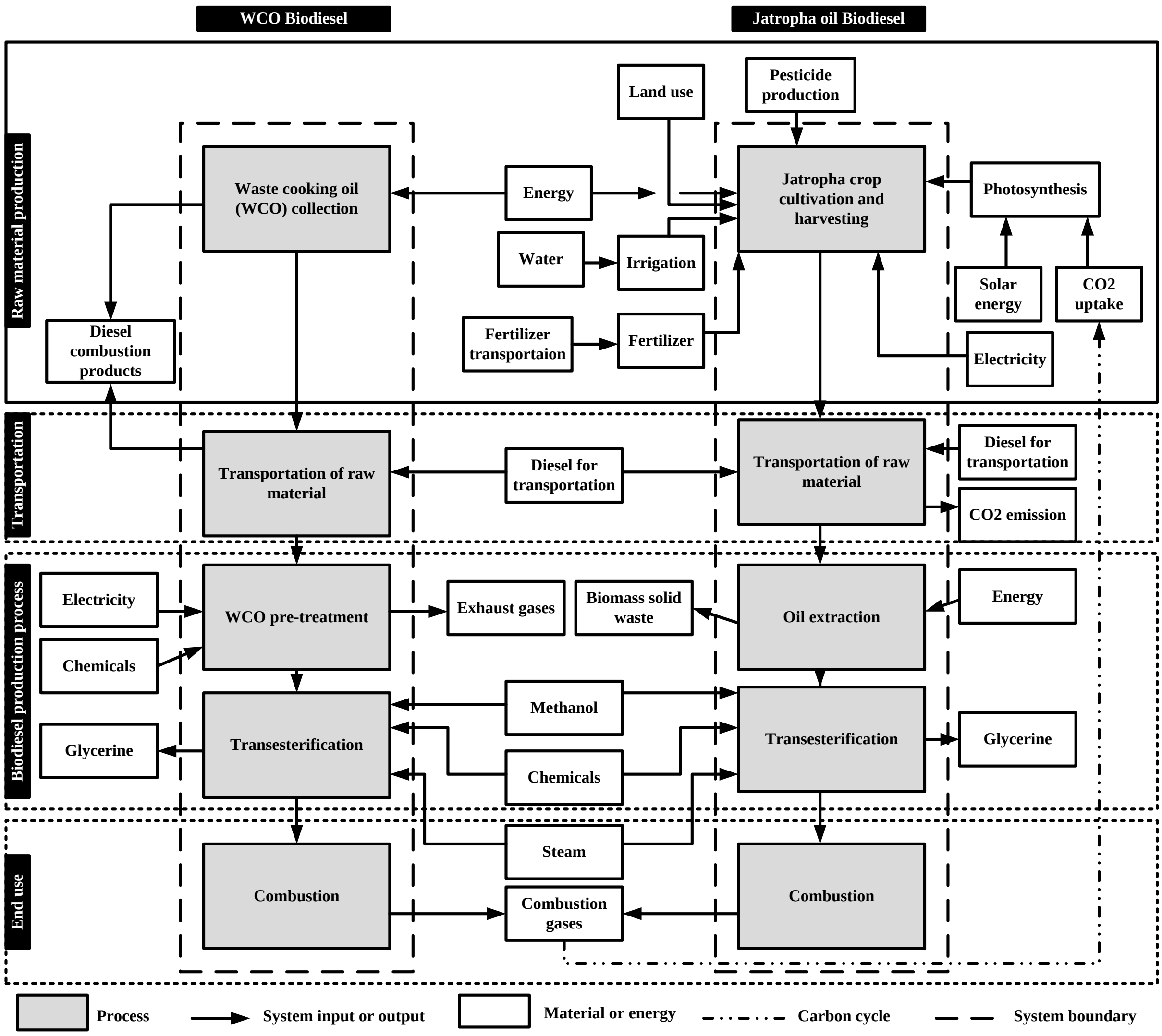


Figure 6.2 Life cycle assessment of biodiesel from waste cooking oil (WCO) and Jatropha oil

6.2.2.3 Life cycle inventory (LCI) and life cycle impact assessment (LCIA)

Inventory requirements for Jatropha crop cultivation, harvesting and seeds oil extraction were adopted from literature (Kumar, Singh et al. 2012). The process simulator results for both cases, Case 1 (production of biodiesel from Jatropha oil) and Case 2 (production of biodiesel from WCO), provided the requirements of material and energy to produce biodiesel and the results are shown in Table 6.1.

Table 6.1 Inventory data for 1.00 t biodiesel production in each process

Stages	Utilities/Raw materials	Case 1	Case 2
Cultivation [a]	Potassium fertilizer (kg/ha)	100	-
	Phosphorous fertilizer (kg/ha)	144	-
	Nitrogen fertilizer (kg/ha)	100	-
	Pesticides used (kg/ha)	2.6	-
	Diesel (for irrigation) (kg/ha)	105	-
Seed oil extraction [b]	Steam (kg/t of seed)	280	-
	Hexane (kg/t of seed)	4	-
	Electricity (kWh/t of seed)	55	-
	Water (kg/t of seed)	12000	-
	Oil extraction efficiency (%)	91	-
	Oil content of seeds (wt. %)	35	-
Biodiesel production	Methanol (t/t of biodiesel)	0.11 [c]	0.2
	Sodium hydroxide (kg/t of biodiesel)	12 [c]	17.2
	Respective oil (t/t of biodiesel)	1.05 [c]	1.07
	Free fatty acid (kg/t of biodiesel)	19.4 [c]	18.2
	Hydrochloric acid (kg/t of biodiesel)	15.8 [c]	12.66
	Sulphuric acid (kg/t of biodiesel)	-	9
	Electricity (kWh/t of biodiesel)	20.78 [c]	50
	Steam (kg/t of biodiesel)	0.66 [c]	1.75
	Biodiesel (t)	1 [c]	1
	Glycerol (kg/t of biodiesel)	103 [c]	152
	Water (kg/t of biodiesel)	0.05 [c]	0.09
Transport	Material (tkm)	50	50
	Collection (tkm)	100	250
Waste	Solid waste (salt)(kg/t of biodiesel)	16 [d]	21.47
	Liquid waste (kg/t of biodiesel)	28.49 [d]	38

[a, b] (Kumar, Singh et al. 2012), [c, d] (case 1) (Sajid, Zhang et al. 2014)

SimaPro 7 was used to perform life cycle studies for both cases. The impact assessment methodology was IMPACT 2002+. The results of this methodology can be expressed in points, which are convenient to interpret (Varanda, Pinto et al. 2011). This methodology connects all results of life cycle studies to damage categories through a midpoint damage approach. There are 14 midpoint categories, which connect the results of life cycle impact to the four damage categories (Jolliet, Margni et al. 2003; Humbert, Schryver et al. 2012). The four damage categories analysed were human health, ecosystem quality, resource and climate change. Following midpoint categories were analysed, the parentheses show their respective midpoint reference substances:

Human toxicity carcinogens HTC (kg_{eq} chloroethylene into air) and human toxicity non-carcinogens HTNC (kg_{eq} chloroethylene into air)

Respiratory inorganics RI (kg_{eq} PM2.5 into air)

Ionizing radiation IR (Bq_{eq} carbon-14 into air)

Ozone layer depletion OLD (kg_{eq} CFC-11 into air)

Photochemical oxidation (PO)/respiratory organics (RO) for human health (kg_{eq} ethylene into air)

Aquatic ecotoxicity AE (kg_{eq} triethylene glycol into water)

Terrestrial ecotoxicity TE (kg_{eq} triethylene glycol into soil)

Terrestrial acidification TA/nitrification N (kg_{eq} SO_2 into air)

Land occupation LO (m^2_{eq} organic arable land.year)

Aquatic acidification AA (kg_{eq} SO_2 into water)

Aquatic eutrophication AE (kg_{eq} PO_4^{3-} into water)

Global warming GW (kg_{eq} CO_2 into air)

Non-renewable energy NRE (MJ Total primary non-renewable energy or kg_{eq} crude oil (860 kg/m^3))

Mineral extraction ME (MJ additional or surplus energy or Kg_{eq} iron (in ore))

6.2.2.4 Data interpretation

A contribution analysis was performed to assess the contribution of each midpoint impact category and comparison for both cases was made. The contributions to damage categories were also analysed to report which raw material and process had more environmental impacts. The study of total environmental impact showed which raw material had more potential to damage environment.

6.3 Results and discussions

6.3.1 Comparison of LCA results of biodiesel production from WCO and Jatropha oil

Relative comparisons between the use of Jatropha oil and WCO as biomass feedstock were analysed for each environmental impact. The larger of two categories was set as 100% and the other was displayed relative to the former, in percentage. The comparative results of LCA are shown in Figure 6.3. As can be seen from Figure 6.3, the use of two different raw materials for biodiesel production has different environmental impacts.

Human toxicity represents all effects on human health besides those of ionizing radiation, photochemical oxidation, inorganic respiratory and ozone layer depletion. Human toxicity carcinogenic and human toxicity non-carcinogenic effects are grouped under this one category. The human toxicity level is decreased by 86.3% with the use of WCO as raw material. This decrease in cumulative toxicological risk and lower potential impacts is associated with the release of chemicals into the environment. Since the Jatropha oil crops cultivation and harvesting requires the use of fertilizers and chemicals. The production of fertilizer and chemicals emits such chemicals into environment and increase the environmental impacts. The use of WCO has the advantage that the raw material has no such requirements.

Respiratory inorganic shows the respiratory effects stemming from the use of inorganic substances in a biodiesel life cycle. The analysis shows that the use of WCO introduces 9.36% respiratory inorganic and it causes less effect on lung or human health.

Ionizing radiations are indicator of waste emissions into water and air. From the results, it is evident that WCO biodiesel contributes 40.10% towards waste emissions into water and air as compared to Jatropha oil biodiesel.

The characterisation factors (CFs) for *ozone layer depletion* represents the emissions to the air. A comparison of results for both biomass feedstocks shows that Jatropha oil biodiesel has less environmental emissions to the air. The use of WCO produces more emissions to air. The use of additional chemicals in WCO pre-treatment could be the potential reason for showing such behaviour.

Respiratory organics introduces respiratory effects, which are due to organic substances. The use of WCO shows less respiratory effects as compared to Jatropha oil biodiesel.

The CFs of *aquatic ecotoxicity* are associated with emissions into soil, water and air. It represents the ecotoxicity effects on fresh water, released during the biodiesel production stages. On comparative bases, WCO biodiesel shows 18.92% effects as compared to Jatropha oil, which is scaled as 100%.

Terrestrial ecotoxicity are the ecotoxicity effects on earth. This includes the emissions to air, water and soil. Since the biodiesel as a fuel reduces overall environmental influences as compared to conventional diesel fuel, therefore the territorial ecotoxicity has negative environmental impact. Moreover, the results show that the production of biodiesel from Jatropha oil is much favourable to reduce the terrestrial environmental impacts.

Land occupation refers to the requirement of land for biodiesel production starting from raw material production to the end use of biodiesel. The results show that the land occupation is much higher in case of Jatropha oil biodiesel as compared to WCO biodiesel. The requirement of land to grow crops for *Jatropha curcas* seeds is the main reason behind such results. Since the whole life cycle study is being carried out, the requirements of land to build biodiesel production plant for WCO biodiesel, adds up a value of 2.73% to land occupation impact category.

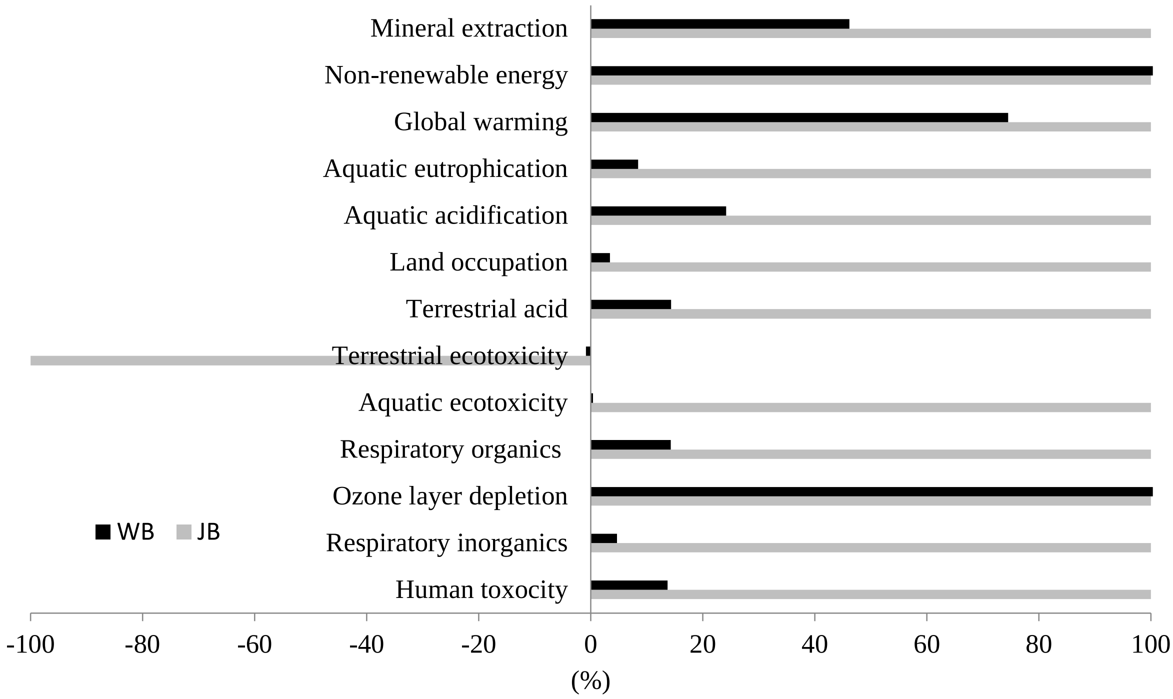


Figure 6.3 Impact categories of waste cooking oil based biodiesel (WB) and Jatropha oil based biodiesel (JB)

The results comparison of *aquatic acidification* show that there is a decrease in pH values of the emissions into water, air and soil for WCO biodiesel and the use of WCO as a biomass feedstock is less harmful to the environment. The effect is 2.42% for WCO biodiesel.

The analysis of *aquatic eutrophication* shows that the use of Jatropha oil as biomass feedstock introduces algal bloom and it reduces the dissolved oxygen in the water. One of the main causes of such phenomenon is the use of fertilizer, the erosion of soil containing nutrients and sewage plant discharges.

Global warming is linked with the emissions of carbon dioxide into air. The results indicate that the use of Jatropha oil introduces more emissions of carbon dioxide into air as compare to WCO use, hence on comparative bases, the use of WCO is more favourable to the environment. The use of WCO as biomass feedstock introduces 29.79% contributions towards global warming.

Non-renewable energy expresses the use of primary energy extracted. The results indicate that there is higher non-renewable energy utilization in case of WCO as biomass feedstock as compared to Jatropha oil. This amount to be 11% higher than that of Jatropha oil. The use of higher energy requirements at plant site could be the possible reasons for such behaviour.

The results of *mineral extraction* show that the use of Jatropha oil plays a major role in mineral extraction as compared to WCO as biomass feedstock. The use of WCO as biomass feedstock contributes 36.92% towards mineral extraction.

6.3.2 Comparisons of damage categories of biodiesel production from WCO and Jatropha oil

The four damage categories analysed were human health, ecosystem quality, climate change and resource. The results are shown in Figure 6.4. The 'human health' damage category is the sum of five midpoint categories. Those are human toxicity, respiratory inorganic, ionizing radiation, ozone layer depletion, and respiratory organics. 'Ecosystem quality' includes six midpoint categories. Those are aquatic ecotoxicity, terrestrial ecotoxicity, terrestrial acid, land occupation, aquatic acidification, and aquatic eutrophication. The damage category 'climate change' includes global warming as midpoint category. The 'resources' damage category is the sum of two midpoints categories which are non-renewable energy and mineral extraction. The use of Jatropha oil as biomass feedstock has higher impacts for human health, ecosystem quality and climate change. The use of WCO has higher impacts for the resources. The values for the respective impacts for WCO are 40.08, 25.70, 29.79 and 110.58%.

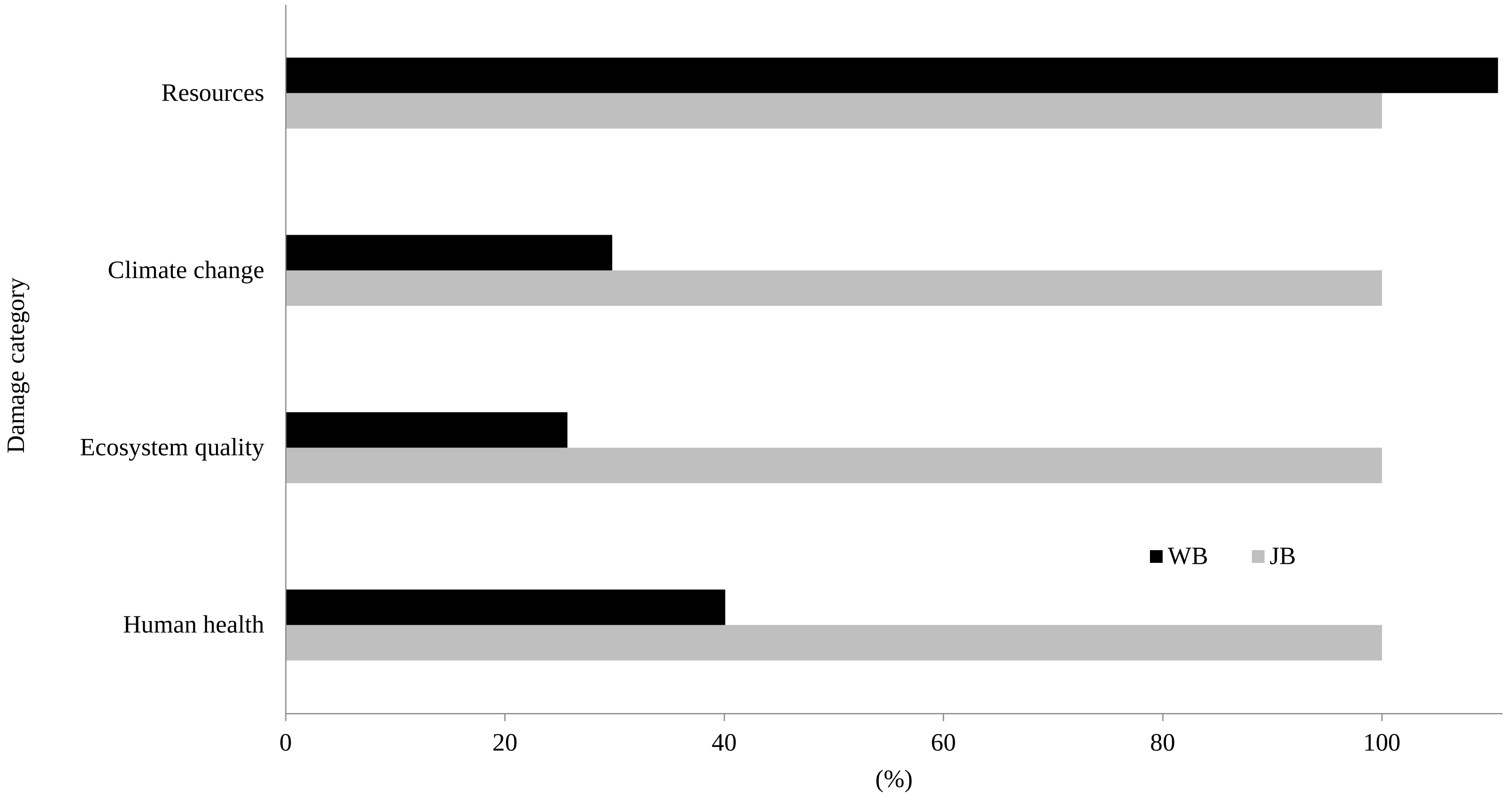


Figure 6.4 Damage categories

A comparison on bases of complete life cycle analysis revealed that which raw material is more environmentally friendly. The results are shown in Figure 6.5. The results of total environmental impacts for WCO and Jatropha oil show that WCO biomass feedstock contributes 26.32% towards environmental impacts when compared with relative 100% of Jatropha oil as biomass feedstock. This shows that the use of WCO as biomass feedstock for biodiesel production is much favourable to the environment.

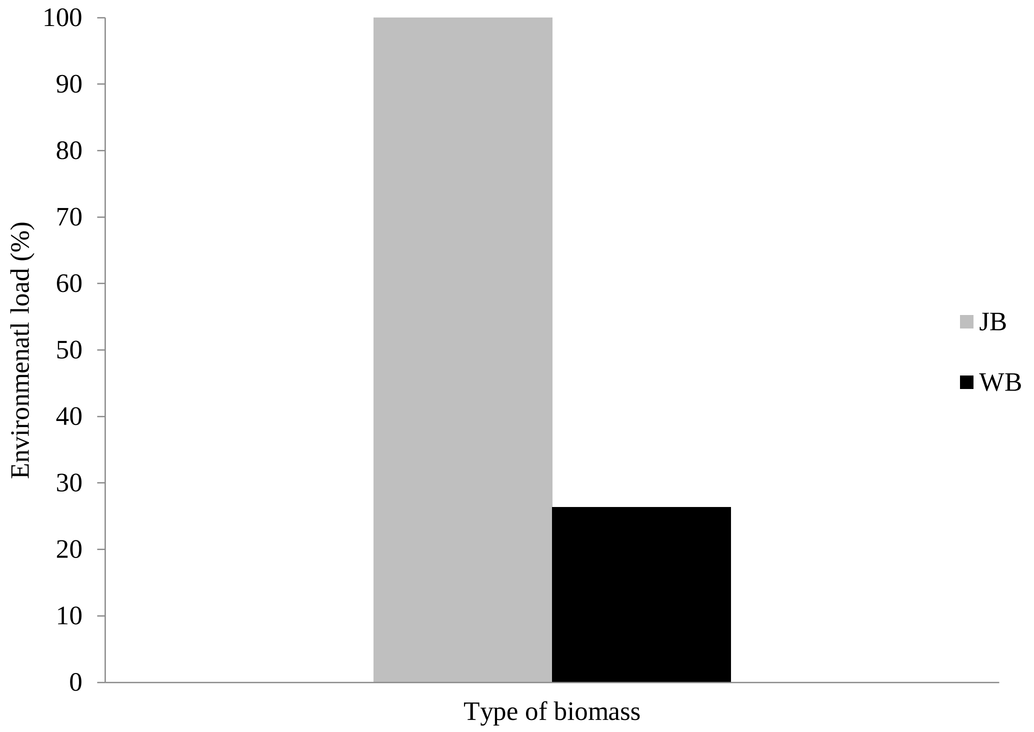


Figure 6.5 Total environmental impact

An analysis of the contributions of the respective processes to the LCA environmental impacts was studied and the results are shown in Figure 6.6 and Figure 6.7. The process contributions of using Jatropha oil are shown in Figure 6.6 and the results of using WCO are shown in Figure 6.7. In Figure 6.6, the results show that for the production of biodiesel from Jatropha oil, biomass cultivation contributes to the highest in each category of environmental impact. This is because the cultivation and harvesting of Jatropha crop needs fertilizer, water, chemicals and land. These materials consume higher energy and mass and their emissions have significant environmental impacts. The auxiliary chemicals required at biodiesel plant to produce biodiesel make the second highest contribution. The production process itself has very less contributions towards environmental impacts.

As shown in Figure 6.7, in case of biodiesel production using WCO, environmental impacts are not much dependent on the raw material preparation phase since biodiesel produced from WCO does not need to use fertilizer, land and water for biomass production. Instead, the chemicals required at plant are contributing highest towards environmental impacts. Moreover, the impact of transport system to collect raw WCO has dominant contributions in each environmental category. These results were based on an average payload distance of 250 tkm and transportation was assumed by road using lorry. The transport distance and collection mechanism is this study was based according to US location where collection mechanism of WCO is well defined. However, the results are highly dependent on regions and their respective collection mechanisms. As evident from Figure 6.7, a change in these transport distances and the type of transport system, could results immense or mild environmental impacts by transport mechanism. A poor collection mechanism would result higher energy consumptions and emissions into environment.

The results of this study are consistent with previously published work. Dufour & Iribarren (2012) analysed the life cycle assessment of four biodiesel production systems using different free fatty acid-rich wastes as raw materials, i.e., vegetable oil, beef tallow, poultry fat, sewage sludge, soybean and rapeseed. Their results showed that environmental impacts of using waste cooking oil were at least comparable to other raw materials. The results in this study also coincide with the observations from another previous work (Niederl-Schmidinger and Narodoslawsky 2008), in which LCA of biodiesel production from tallow and used cooking oil were investigated and compared. They found environmental impacts were lower in case of using used cooking oil as raw biomass material and biodiesel produced from used cooking oil was more environmentally friendly. However these studies did not compare the environmental impacts of waste cooking oils with those of inedible oils. The present study contributes in existing literature by discussing such aspects.

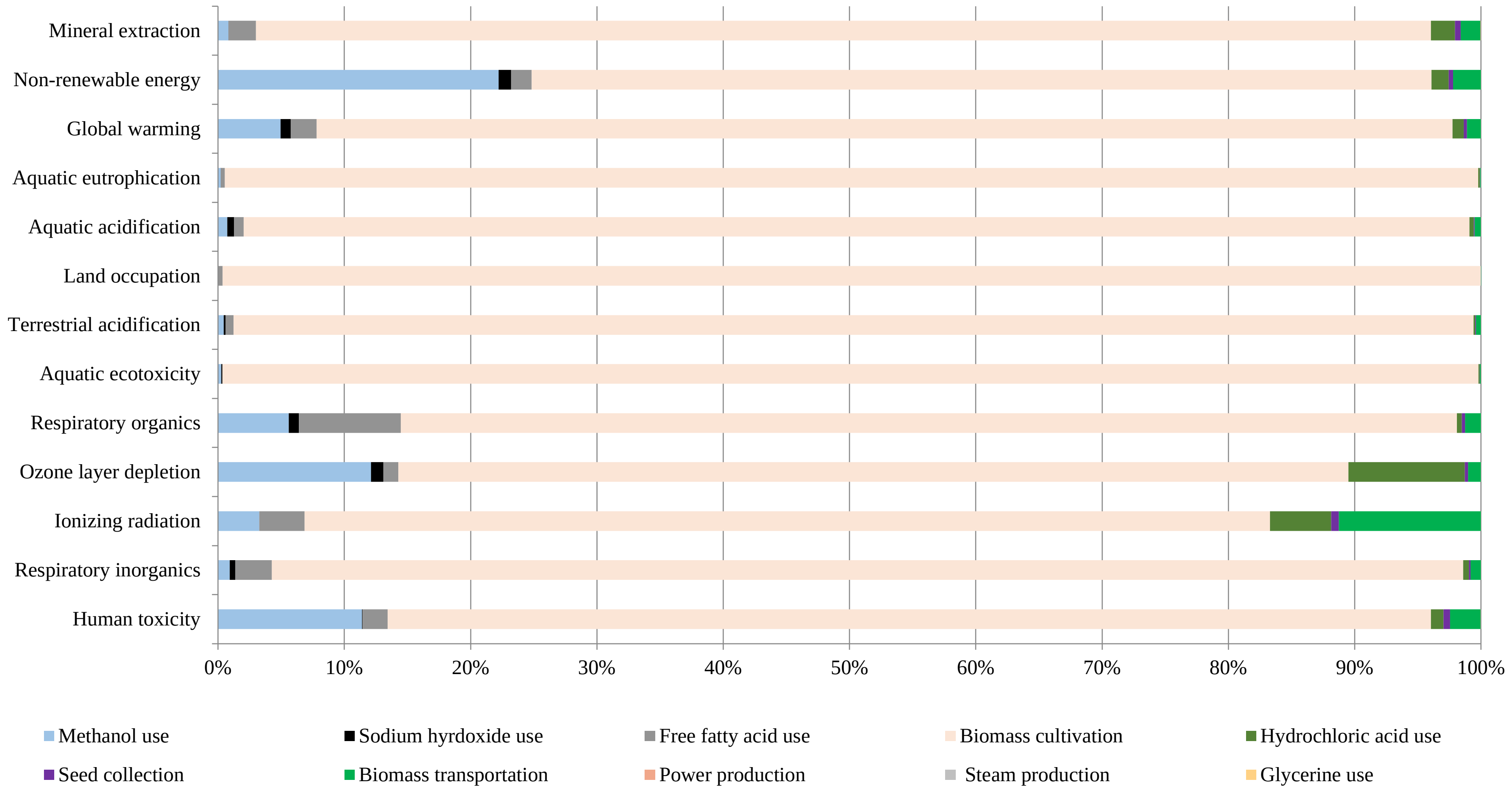


Figure 6.6 Relative contributions of technological process elements to the LCA of biodiesel from Jatropha oil

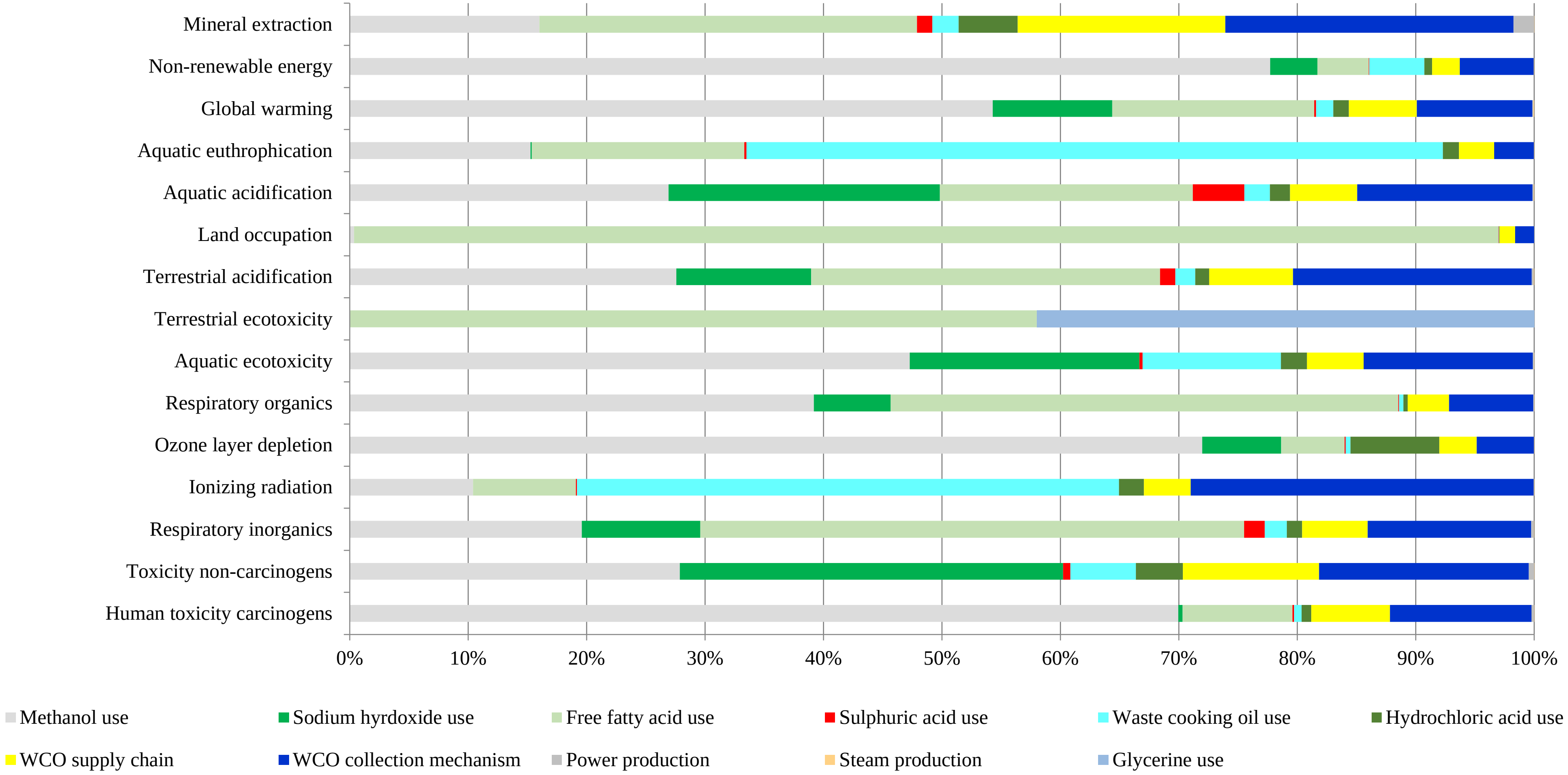


Figure 6.7 Relative contributions of technological process elements to the LCA of biodiesel from WCO

6.4 Conclusions

Alkali-catalysed process was chosen to analyse the environmental impacts of biodiesel production from two different raw materials, non-edible Jatropha oil and waste cooking oil (WCO). The environmental impacts generated by each process were analysed using life cycle assessment (LCA) as a tool. It was found that, on a complete life cycle bases, the biodiesel produced from WCO has less impacts on the environment because of its less demanding raw material. The study showed that the preparation of raw material for WCO requires no special energy other than collecting it from various sources. The production of non-edible Jatropha oil requires the use of land though the soil fertility requirements are less demanding compared to those for edible oil source. Moreover, the production of Jatropha oil takes time to grow crops but WCO is immediately available to use. However, the sources of WCO are scattered and the collection of WCO from these sources requires higher transportation coverage. From the standpoint of production, the study showed that the production process of WCO utilizes higher energy contents and more chemicals. From the environmental perspective, the production process from Jatropha oil produces less environmental impacts as compared to those from WCO process. The study revealed that the production of biodiesel using WCO as raw material is more environmentally friendly. However, other than the study of the environmental impacts, the decision of using either raw material should also be based on the process economics analysis.

6.5 References

Abbaszaadeh, A., B. Ghobadian, et al. (2012). "Current biodiesel production technologies: A comparative review." Energy Conversion and Management **63**: 138-148.

Achten, W. M. J., L. Verchot, et al. (2008). "Jatropha bio-diesel production and use." Biomass and Bioenergy **32**(12): 1063-1084.

Ali, M. H., M. Mashud, et al. (2013). "Biodiesel from Neem Oil as an Alternative Fuel for Diesel Engine." Procedia Engineering **56**: 625-630.

Ashraful, A. M., H. H. Masjuki, et al. (2014). "Production and comparison of fuel properties, engine performance, and emission characteristics of biodiesel from various non-edible vegetable oils: A review." Energy Conversion and Management **80**: 202-228.

Atabani, A. E., A. S. Silitonga, et al. (2013). "Non-edible vegetable oils: A critical evaluation of oil extraction fatty acid compositions, biodiesel production, characteristics, engine performance and emissions production." Renewable and Sustainable Energy Reviews **18**: 211-245.

Banković-Ilić, I. B., O. S. Stamenković, et al. (2012). "Biodiesel production from non-edible plant oils." Renewable and Sustainable Energy Reviews **16**(6): 3621-3647.

Bharathiraja, B., M. Chakravarthy, et al. (2014). "Biodiesel production using chemical and biological methods - A review of process, catalyst, acyl acceptor, source and process variables." Renewable and Sustainable Energy Reviews **38**: 368-382.

Borugadda, V. B. and V. V. Goud (2012). "Biodiesel production from renewable feedstocks: Status and opportunities." Renewable and Sustainable Energy Reviews **16**(7): 4763-4784.

Cho, S., J. Kim, et al. (2015). "Incentives for waste cooking oil collection in South Korea: A contingent valuation approach." Resources, Conservation and Recycling **99**: 63-71.

Cynthia, O.-B. and K. T. Lee (2011). Feasibility of Jatropha Oil for Biodiesel: Economic Analysis. World Renewable Energy Congress – Sweden, Linköping, Sweden, Linköping University Electronic Press, Linköpings universitet.

Dhar, A. and A. K. Agarwal (2014). "Performance, emissions and combustion characteristics of Karanja biodiesel in a transportation engine." Fuel **119**: 70-80.

Dufour, J. and D. Iribarren (2012). "Life cycle assessment of biodiesel production from free fatty acid-rich wastes." Renewable Energy **38**(1): 155-162.

Energy, U. (2014). US Energy Information Administration - Independent Statistics and Analysis.

Farrell, S. and E. Cavanagh (2014). "An introduction to life cycle assessment with hands-on experiments for biodiesel production and use." Education for Chemical Engineers **9**(3): e67-e76.

Frischknecht, R., N. Jungbluth, et al. (2007). Overview and Methodology. Dubendorf, Swiss Centre for Life Cycle Inventories.

Gopal, K. N., A. Pal, et al. (2014). "Investigation of emissions and combustion characteristics of a CI engine fueled with waste cooking oil methyl ester and diesel blends." Alexandria Engineering Journal **53**(2): 281-287.

Haas, M. J., A. J. McAloon, et al. (2006). "A process model to estimate biodiesel production costs." Bioresource Technology **97**(4): 671-678.

Hasibuan, S., A. Ma'ruf, et al. (2009). "Biodiesel from low grade used frying oil using esterification transesterification process." Makara journal of science **13**(2): 105-110.

Hou, J., P. Zhang, et al. (2011). "Life cycle assessment of biodiesel from soybean, jatropha and microalgae in China conditions." Renewable and Sustainable Energy Reviews **15**(9): 5081-5091.

Huerga, I. R., M. S. Zanuttini, et al. (2014). "Biodiesel production from Jatropha curcas: Integrated process optimization." Energy Conversion and Management **80**(0): 1-9.

Humbert, S., A. D. Schryver, et al. (2012). IMPACT 2002+: User Guide, Quantis International.

Jolliet, O., M. Margni, et al. (2003). "IMPACT 2002+: A new life cycle impact assessment methodology." The International Journal of Life Cycle Assessment **8**(6): 324-330.

Kaewcharoensombat, U., K. Prommetta, et al. (2011). "Life cycle assessment of biodiesel production from jatropha." Journal of the Taiwan Institute of Chemical Engineers(42): 454-462.

Kiwjaroun, C., C. Tubtimdee, et al. (2009). "LCA studies comparing biodiesel synthesized by conventional and supercritical methanol methods." Journal of Cleaner Production **17**(2): 143-153.

Kulkarni, M. G. and A. K. Dalai (2006). "Waste cooking oil - An economical source for biodiesel: a review." Ind. Eng. Chem. Res. **45**(9): 2901-2913.

Kumar, S., J. Singh, et al. (2012). "A comprehensive life cycle assessment (LCA) of Jatropha biodiesel production in India." Bioresource Technology **110**: 723-729.

Lu, H., Y. Liu, et al. (2009). "Production of biodiesel from Jatropha curcas L. oil." Computers and Chemical Engineering **33**(5): 1091-1096.

M, K. and G. D (2014). "Feasibility evaluation of a biodiesel plant fed by recycled edible oils comparing two alternative production technologies." Global NEST Journal: in press.

Marchetti, J. M., V. U. Miguel, et al. (2008). "Techno-economic study of different alternatives for biodiesel production." Fuel Processing Technology **89**(8): 740-748.

Mohammadshirazi, A., A. Akram, et al. (2014). "Energy and cost analyses of biodiesel production from waste cooking oil." Renewable and Sustainable Energy Reviews **33**: 44-49.

Morais, S., T. M. Mata, et al. (2010). "Simulation and life cycle assessment of process design alternatives for biodiesel production from waste vegetable oils." Journal of Cleaner Production **18**(13): 1251-1259.

Naima, K. and A. Liazid (2013). "Waste oils as alternative fuel for diesel engine: A review." Journal of Petroleum Technology and Alternative Fuels **4**(3): 30-43.

Niederl-Schmidinger, A. and M. Narodoslawsky (2008). "Life Cycle Assessment as an engineer's tool?" Journal of Cleaner Production **16**(2): 245-252.

Omer, A. M. (2008a). "Energy, environment and sustainable development." Renewable and Sustainable Energy Reviews **12**(9): 2265-2300.

Omer, A. M. (2008b). "Green energies and the environment." Renewable and Sustainable Energy Reviews **12**(7): 1789-1821.

Phan, A. N. and T. M. Phan (2008). "Biodiesel production from waste cooking oils." Fuel **87**(17-18): 3490-3496.

Puhan, S., N. Vedaraman, et al. (2005). "Mahua oil (Madhuca Indica seed oil) methyl ester as biodiesel-preparation and emission characterstics." Biomass and Bioenergy **28**(1): 87-93.

Raja, S. A., D. S. R. Smart, et al. (2011). "Biodiesel production from Jatropha oil and its characterization." Research Journal of Chemical Sciences **1**(1): 81-87.

Ramos, T. R. P., M. I. Gomes, et al. (2013). "Planning waste cooking oil collection systems." Waste Management **33**(8): 1691-1703.

Refaat, A. A. (2010). "Different techniques for the production of biodiesel from waste vegetable oil." International Journal of Environmental Science and Technology **7**(1): 183-213.

Royon, D., M. Daz, et al. (2007). "Enzymatic production of biodiesel from cotton seed oil using t-butanol as a solvent." Bioresource Technology **98**(3): 648-653.

Sahoo, P. K. and L. M. Das (2009). "Process optimization for biodiesel production from Jatropha, Karanja and Polanga oils." Fuel **88**(9): 1588-1594.

Sajid, Z., Y. Zhang, et al. (2014). "Process design and probablistic economic risk analysis of bio-diesel production " under review.

Shah, M., S. Ali, et al. (2014). "Catalytic conversion of jojoba oil into biodiesel by organotin catalysts, spectroscopic and chromatographic characterization." Fuel **118**(0): 392-397.

Singhabhandhu, A. and T. Tezuka (2010). "Prospective framework for collection and exploitation of waste cooking oil as feedstock for energy conversion." Energy **35**(4): 1839-1847.

Usta, N., B. Aydogan, et al. (2011). "Properties and quality verification of biodiesel produced from tobacco seed oil." Energy Conversion and Management **52**(5): 2031-2039.

Varanda, M. G., G. Pinto, et al. (2011). "Life cycle analysis of biodiesel production." Fuel Processing Technology **92**(5): 1087-1094.

Zhang, Y., M. A. Dube, et al. (2003). "Biodiesel production from waste cooking oil: 2. Economic assessment and sensitivity analysis." Bioresource Technology **90**(3): 229-240.

Chapter 7

7 Conclusions and recommendations

Authorship and contributorship

This chapter concludes the findings based on the developed methodologies presented in this thesis about process economics and the environmental sustainability of biodiesel fuel. It also provides recommendations for future research in this domain and discusses the contributions and innovations of this thesis to the current literature. The first author, Zaman Sajid, summarised the conclusion, developed and proposed the recommendations for future work and drafted the chapter. The co-authors, Drs. Faisal Khan and Yan Zhang, supervised the whole process and provided valuable comments and feedback to improve the chapter.

7.1 Conclusion

In this study, the economic viability and environmental sustainability of biodiesel were investigated. The limitations of current biodiesel process economic studies were identified along with the current techno-economic challenges in the study of biodiesel process economics. An integrated approach was developed to identify the qualitative and quantitative interdependence of biodiesel performance risk factors. The practical applications of such approach and its importance were highlighted using biodiesel case studies. The models presented in this study would assist the biodiesel process industry, owners, managers and investors to identify key risk factors in biodiesel plant design, process and operations. This thesis also demonstrated the level of uncertainty over the time period of biodiesel plant start-up and operations. Additionally, a life cycle thinking approach was used to present the environmental sustainability of biodiesel fuel. The approach helped to quantify contributions of biodiesel production and use to address global warming issues, ecosystem disruptions and core ecological issues. The specific conclusions of this thesis were:

7.1.1 Development of probabilistic cost risk analysis approach

To perform biodiesel process economic analysis, various cost factors are involved. These are: variable cost, fixed cost, total capital investment, total cost of biodiesel production and the annual operating cost. The process design and simulations performed identified that among these cost components associated with biodiesel production on an industrial scale, the cost of raw material significantly affects biodiesel process economics. The reactor to produce biodiesel through chemical conversion has the highest risk of cost escalation associated with its cost estimation. The analysis in this thesis identified that the cost estimation using traditional process economics techniques is either overestimated or underestimated. Therefore, the study concluded that the cost estimated through the proposed approach of probabilistic process economic analysis is more precise than the traditional process economic analysis techniques available in literature. The analysis also showed that the inclusion of a monetary carbon tax can make biodiesel projects economical ones. The integration of the uncertainty in cost data and process contributed significantly to process design decision-making.

7.1.2 Biodiesel key performance indicators (KPIs) and their management

This thesis discussed the qualitative and quantitative key performance indicators (KPIs) for a biodiesel facility. The findings of the proposed interdependency model highlighted the fact that in biodiesel risk factors, biodiesel operational safety is the key risk factor to evaluate, monitor and improve the performance of a biodiesel production plant. The findings also indicated that the environmental risk factor has an impact on both natural resource depletion and occupational health. Given the complexity of relationships among risk categories of process, operations and design, a Bayesian Network (BN) approach identified that there exists a strong relationship between occupational health and plant safety, and hence this conclusion helps to allocate financial resources and develop KPI management for a biodiesel plant in an effective way.

7.1.3 Estimation of Process Value at Risk (VaR)

In this study, a model was presented to assess the process economics using value at risk (VaR). The developed methodology analysed the interdependency among biodiesel cost related risk factors. To illustrate the application, a case study was undertaken to quantify financial risk for a biodiesel facility. The case study results showed that the return period for a biodiesel production plant varies with the maximum acceptable loss value and the given confidence level. The analysis also concluded that the payback period from traditionally available process economic techniques is misleading as it does not consider the impact of various risk factors on process economics. This technical deficiency has been diminished by the proposed methodology in this thesis.

7.1.4 Environmental sustainability of biodiesel production and process

The severe environmental impacts of fossil-based fuels can be mitigated using biodiesel. The use of biodiesel as an alternate to fossil-based fuel would also help to reduce dependency on natural resources and to preserve the environment by controlling greenhouse gas emissions. The simulations performed to design a biodiesel process plant followed by life cycle studies concluded that the use of waste cooking oil (WCO) instead of inedible jatropha oil as biomass feedstock decreases the human toxicity level significantly. The use of chemicals and the need of high energy in the WCO pre-treatment process introduce higher emissions than does extracting jatropha oil from jatropha *curcas* by mechanical pressing. In terms of global warming, the results concluded that WCO has fewer environmental effects than jatropha oil as a biomass feedstock. In conclusion, the study indicated that on a life cycle basis the use of WCO instead of jatropha oil as biomass feedstock is more favourable to the environment. However, this research also proposed an effective collection mechanism and supply chain management for WCO.

7.2 Contributions and Research Innovation

This thesis contributes to the development of innovative scientific and engineering knowledge in the field of sustainable energy, and in particular, bioenergy. It proposed innovative, engineering-based, technological methodologies in the areas of economic and environmental sustainability of bio-energy systems. Research on biodiesel sustainability has been performed for more than two decades; however, the research area identified in this thesis is a new one. A comprehensive review produced no studies which included the quantification of cost-risk, associated vulnerabilities and performance management system in the biodiesel industry. In fostering innovation in the biodiesel chemical industry, the first step is to determine if the proposed biodiesel technology is commercially viable. In engineering, this analysis is called "techno-economic" analysis of a biodiesel system. In this analysis, different biodiesel cost variables are analysed before an innovation in biodiesel production is introduced into the marketplace. Such assessments help to commercialize the technology and foster the achievement of the economic goals of the society by introducing a new alternate fuel into society. Since food is a vital need of human beings, the use of edible oils as biodiesel feedstock has resulted in a debate on this use of energy vs food production (Lam, Tan et al. 2009). This thesis performed a techno-economic analysis of biodiesel production system using inedible oil as feedstock to address this debate. Additionally, this thesis contributed to the existing literature by providing a sustainability analysis for the biodiesel industry and serves as roadmap to perform future research in the arena of biodiesel supply chain management and resource allocation. In doing so, a brief description of four major contributions made by this thesis in the existing literature and their respective research innovations are presented below:

7.2.1 Economic risk analysis of biodiesel plant

The existing literature on biodiesel process economics performs economic analysis and reports the expected profit based on estimated cost and estimated revenue.

However, these analyses do not present reliable cost and revenue data since their uncertainties influence the accuracy of the process economics and subsequently can alter the decisions being made on their bases. Therefore, there was a need to perform a study which could identify the level of uncertainty in cost and revenue data. In order to address this research gap, this thesis proposed a robust model to estimate the uncertainties present in cost and revenue data, and identified the cost-escalation risk associated with such uncertainties. Moreover, the model also identified the most and the least cost-vulnerable production units in a biodiesel plant. More details were presented in Chapter 3 of the thesis.

7.2.2 Uncertainties due to technological innovations

Today, biodiesel technology is evolving faster than it was a decade ago and in this scenario, the optimal decisions about the use of biodiesel should not be solely based on its techno-economic studies. Instead, there is a need to develop a biodiesel performance risk management system, which would help to study the performance of a biodiesel system affected by various risk factors. Generally speaking, these risk factors include risks associated with the biodiesel process, design and operations. In order to develop and sustain this risk management system, first there is a need to identify in-depth details of such risk factors and secondly, the developments of a methodological framework which could not only identify their impacts on the performance of biodiesel systems but could also assess their interdependencies.

In this regard, this thesis contributes to the existing literature by proposing an innovative integrated technique, which studied quantitative and qualitative interdependency of risk factors affecting the performance of a biodiesel production system. More details were provided in Chapter 4.

7.2.3 Simulation and modelling of financial engineering tools in process engineering

In today's energy seeking world, the research in bio-energy has introduced various technologies, raw material, and processes to produce bio-energy. However, to scale up such technologies on an industrial scale, an investor faces many factors affecting the cost-benefit analysis of these projects. These factors are environmental changes, process design reliability, cost overrun, operational and equipment robustness and many more (see Chapter 4 for more details). Since such factors are dynamic in nature, there is a need to develop a dynamic approach to deal with these challenges. A Bayesian Network (BN) approach has been presented in this thesis to study the impact of these factors on overall performance of a biodiesel system. Since an investor would likely wants to know the impact of cost risk factors on returns, in this regard in Chapter 5, a methodological framework has been presented based on cost related risk factors. Chapter 5 provided the effects of cost related risk factors on the performance of a biodiesel system, and outlined a new process economic model. The model was based on modelling a financial engineering tool, called value at risk (VaR), which studies biodiesel process economics in an innovative way. The model incorporated the interdependencies of various biodiesel cost risk factors which were identified through literature and their impacts on biodiesel process economics. In developing this methodology, the qualitative and quantitative relationships among various biodiesel cost related risk factors were defined, and the qualitative and quantitative nature of these risk factors was integrated with an objective risk analysis approach. This identified the most significant risk factors in biodiesel process economics study. The developed model helps managers and investors in biodiesel operations to make financial risk decisions and assists in the study of the overall performance of a biodiesel production system.

7.2.4 Environmental life cycle assessment of biodiesel

Other than the economic and social pillars, the sustainability of biodiesel is also dependent on its environmental pillar, which identifies the environmental impacts of the production and use of biodiesel. Various biodiesel production systems generate different by-products, consume various chemicals and affect ecosystem ecology. Therefore, the results of life cycle assessment (LCA) are significantly dependent on the methods used in LCA studies for the preparation and treatment of these various chemicals and different by-products (Bernesson, Nilsson et al. 2006, Menichetti and Otto 2008). Hence, a comparison of environmental impacts of two distinct biodiesel technologies and raw materials is only possible when the analysis is performed on a unique material and energy basis. In this regard, Chapter 6 provided an LCA of biodiesel production from two different technologies and raw materials, and compared environmental impacts of these technologies and raw materials. The results help to develop an improved biodiesel environmental management system which could improve the efficiency of biodiesel, decision-making for biodiesel stakeholders and communications for biodiesel policy making.

To summarize, this thesis contributed by developing new methodologies for biodiesel process economics and assessing the environmental impacts of biodiesel production and process using different biomass feedstock.

7.3 Recommendations

The present work introduces innovative concepts in biodiesel process economics and process design. It also overcomes the limitation of existing process techniques in the field of sustainable process and environmental engineering. However, this study can be extended further by addressing the main limitation of this work, as presented in the sections below:

7.3.1 Integration of Carbon tax and probabilistic economic risk analysis

This study shows that the proposed probabilistic economic risk analysis methodology and Monte Carlo Simulation approach can identify the true uncertainties present in the cost and revenue data of a biodiesel process economics study. The probabilistic risk analysis on revenue data was performed considering direct and indirect revenues only (see Section 3.4.2). However, as presented in Table 3.5, the use of biodiesel instead of petroleum-based diesel can provide a tax saving of USD $ 0.15 million in carbon tax. It is recommended to perform probabilistic risk analysis on revenue data considering these environmental benefits.

7.3.2 Approximation of uncertainty modelling and distribution

The probabilistic risk analysis presented in Section 3.4 used the triangular distributions to perform Monte Carlo Simulation on both cost and revenue data. Although upper, lower and the most likely values make triangular distribution the most appropriate distribution to perform simulations for cost and revenue data, it is recommended to perform the analysis using other distributions such as normal distribution, since actual cost and revenue data may fall outside the limits of the upper and lower values used in triangular distribution.

7.3.3 Development of binary contextual relationships

In the application of ISM methodology (see Section 4.1), the binary contextual relationships among various risk factors were developed using experts' opinions. In this study, the experts were a university research group working under the guidance of a senior university professor. Although, based on their level of qualifications and research expertise, research group was able to develop an initial relationship among risk factors, it is recommended to widen the binary contextual relationship by also considering opinions from field experts in the area of process design, managers and stakeholders of biodiesel production, process and operational personnel.

7.3.4 Comprehensiveness of risk factors

The Table 4.1, Table 4.2 and Table 4.3 enlisted various risk factors for process, design and installation and operations categories for a biodiesel facility. These comprehensive lists were developed using a detailed literature review and therefore are generic in nature. Though these Tables cover many risk factors associated with their respective categories, it is recommended to expand the respective list as new risk factors are discovered in future studies. This work presents methodologies based on bio-diesel production systems. However since risks have their due importance in other energy production systems, it is recommended to implement these methodologies on other energy systems such as wind energy, solar energy, geothermal energy etc. while performing their economics and environmental impact studies.

7.3.5 Commercial tool for complex network modelling

The proposed approach in Section 4.3 used a case study of five risk factors, presented in Table 4.4. The calculations of CPTs using BN as presented in Figure 4.4 were performed in Excel; however, the results would be difficult to obtain using Excel when the number of risk factors increases, as this would develop a complex network. In this case, the use of Genie modeller – decision modelling software provided by Bayes Fusion LLC, is recommended to develop a BN model of the problem using CPTs. The Genie modeller can be accessed at https://www.bayesfusion.com/genie-modeler

7.3.6 Development of VaR model using revenue risk factors

In the application of the proposed VaR methodology, as presented in Section 5.2, it was assumed that total cost is the only uncertain variable and is influenced by its relevant risk factors and that the revenue is a certain variable, not influenced by any risk factors. Since cost and revenue both affect the overall profit, it is recommended to implement the proposed methodology to model VaR by considering the variability in both cost and revenue. This would include the study of the interdependency of revenue risk factors using a BN modelling approach and the combined impact of cost-related and revenue-related risk factors on VaR.

7.3.7 Integration of logistic risk factors and VaR modelling

The process VaR model presented in Section 5.2 only considered the risk associated with cost variables. In order to develop an effective supply chain management system for a biodiesel production system, there is a need to include logistic risks in the study. Therefore, it is recommended to include the impact of logistic risks in VaR modelling. The results would be beneficial in planning, implementing, and controlling the availability of biomass and biofuels. The recommended work would also help to reduce vulnerability and would ensure continuity of the biomass to the biofuel industries and the biofuels to the end-users.

7.3.8 Development of probabilistic social risk analysis model

The sustainability of a product is based on the fact that the product provides economic, environmental and social benefits. This work focused on the economic and environmental aspects of biofuels; however, it is recommended to develop a methodology for probabilistic social risk analysis of biofuels as future research work.

7.4 References

Bernesson, S., D. Nilsson and P.-A. Hansson (2006). "A limited LCA comparing large and small scale production of ethanol for heavy engines under Swedish conditions." Biomass and Bioenergy 30 (1): 46-57.

Lam, M. K., K. T. Tan, K. T. Lee and A. R. Mohamed (2009). "Malaysian palm oil: Surviving the food versus fuel dispute for a sustainable future." Renewable and Sustainable Energy Reviews 13 (6–7): 1456-1464.

Menichetti, E. and M. Otto (2008). "Energy balance and greenhouse gas emissions of biofuels from a life-cycle perspective." Biofuels: Environmental Consequences and Interactions with Changing Land Use. Proceedings of the Scientific Committee on Problems of the Environment (SCOPE) International Biofuels Project Rapid Assessment, Ithaca NY: University of Cornell: 81-109.