Multi-Criteria Decision-Making in Whole Process Design

A thesis submitted by

Richard Edgar Hodgett

For the degree of Doctor of Philosophy

School of Chemical Engineering and Advanced Materials

Newcastle University

January 2013

Abstract

In recent years, the chemical and pharmaceutical industries have faced increased development times and costs with fewer novel chemicals being discovered. This has resulted in many companies focusing on innovative research and development as they consider this key to business success. In particular, a number of leading industrial organisations have adopted the principles of Whole Process Design (WPD). WPD considers the optimisation of the entire product development process, from raw materials to end product, rather than focusing on each individual unit operation. The complexity involved in the implementation of WPD requires rationalised decision-making, often with limited or uncertain information.

This thesis assesses the most widely applied methods in Multi-Criteria Decision Analysis (MCDA) in conjunction with the results of two interviews and two questionnaires that identified the industrial requirements for decision-making during WPD. From the findings of this work, a novel decision-making methodology was proposed, the outcome of which allows a decision-maker to visually interpret their decision results with associated levels of uncertainty. To validate the proposed methodology, a software framework was developed that incorporates two other decision-making approaches, the Analytical Hierarchy Process (AHP) and ELimination Et Choix Traduisant la REalité trois (ELECTRE III). The framework was then applied to a number of industrial case studies to validate the application of the proposed methodology.

Keywords: Multi-Criteria Decision Analysis (MCDA); Multi-Attribute Range Evaluations (MARE); Whole Process Design (WPD); Uncertainty.

Acknowledgements

I would like to sincerely thank my academic supervisors, Prof. Gary Montague and Prof. Elaine Martin OBE FREng, for firstly giving me the opportunity to complete my postgraduate studies and secondly for their support, encouragement and guidance throughout the last four years. I would particularly like to thank Elaine for the tremendous effort she put into reading and advising me on my thesis and journal papers. I would also like to thank my industrial supervisor Dr. Mark Talford and everyone at Britest Limited for their support and financial funding which has enabled me to complete my research. Similarly, I would like to thank the Engineering and Physical Sciences Research Council (EPSRC) and Chemistry Innovation for their financial support. I am thankful to Dr. Dave Compton, Zac Meadows, Andrew Rutter and David Robertson for their insight into industrial decision-making.

I owe a great deal to my friends and colleagues in my office and research group. In particular, I'd like to express my gratitude to Dr. Aruna Manipura and Dr. Chris O'Malley, Aruna for challenging my mind and Chris for challenging my liver. I would also like to thank Louise Hogg for her support and encouragement. Last but no means least, I would like to thank my family, including my dad Stephen for his continued support, from when I was a little terror until now (a big terror?) and my sister Sarah for her kindness and uplifting humour. Above all, I am forever grateful to my mum, Susan, for her loving guidance, encouragement and support. Without her I would not be writing this thesis.

Table of Contents

1 Thesis Introduction and Overview ... 1

1.1 Thesis Motivation ... 1

1.2 Aims and Objectives ... 5

1.3 Research Questions ... 5

1.4 Industrial Relationship ... 6

1.5 Thesis Structure ... 7

2 Methods and Techniques ... 9

2.1 Introduction ... 9

2.2 Decision-Making Techniques ... 9

2.2.1 History of Decision-Making Techniques ... 10

2.2.2 Decision-Making Processes ... 17

2.2.3 Multi-Objective Optimisation ... 21

2.2.4 Multi-Attribute Methods ... 31

2.2.5 Outranking Methods ... 36

2.2.6 Other Techniques ... 41

2.3 Behavioural Decision-Making ... 46

2.3.1 Intuition and Rational Thought ... 46

2.3.2 Group Decision-Making ... 48

2.3.3 Modelling Irrational Behaviour and Uncertainty ... 49

2.4 Chemical Decision Literature ... 51

2.4.1 Multi-Objective Optimisation Applications ... 52

2.4.2 Multi-Attribute and Outranking Applications ... 54

2.5 Conclusions ... 56

2.5.1 Methods and Uncertainty ... 56

2.5.2 Methods used in Process Design ... 58

3 Industrial Requirement ... 59

3.1 Introduction 59

3.2 Interviews 59

3.2.1 Robinson Brothers Limited 60

3.2.2 BP 61

3.2.3 Interview Outcomes 63

3.3 Questionnaires 64

3.3.1 Techniques currently used for decision-making in industry 65

3.3.2 Decisions made throughout WPD 67

3.3.3 Requirements for a Decision-Making Framework 68

3.4 Conclusions 72

3.4.1 Decision-making Techniques 73

3.4.2 Whole Process Design Decisions 73

3.4.3 Framework Requirements 73

4 Materials and Methods 76

4.1 Introduction 76

4.2 Decision-Making in Whole Process Design 76

4.3 Multi-Attribute Range Evaluations 77

4.4 Evaluation Strategy 80

4.5 ChemDecide Framework 80

4.5.1 Framework Overview 82

4.5.2 Logical Overview 83

4.5.3 Implementation Overview 94

4.6 Conclusions 96

5 Case Studies 98

5.1 Introduction 98

5.2 Route Selection (Robinson Brothers) 99

5.3.1 AHP Analysis 100

5.3.2 MARE Analysis 102
5.3.3 RANK Analysis 104
5.3.4 Evaluation 105
5.3.5 Conclusions 106
5.3 Degassing Methodology Selection (GSK) 107
5.3.1 AHP Analysis 108
5.3.2 MARE Analysis 110
5.3.3 RANK Analysis 112
5.3.4 Evaluation 114
5.3.5 Post Analyses Interview 117
5.3.6 Conclusions 118
5.4 Premix Equipment Selection (FFIC) 118
5.4.1 AHP Analysis 119
5.4.2 MARE Analysis 121
5.4.3 RANK Analysis 124
5.4.4 Evaluation 126
5.4.5 Post Analyses Interview 129
5.4.6 Conclusions 130
5.5 User Evaluation of the Framework 130
5.5.1 Inputs 131
5.5.2 Outputs 132
5.5.3 Uncertainty 132
5.5.4 Analysis Time 132
5.5.5 Overall Evaluation 132
5.5.6 Future Requirements 133
5.5.7 Conclusions of the User Evaluation 133
5.6 Conclusions 134

6 Case Study Discussion 136
6.1 Introduction 136
6.2 Source of the inconsistencies in the case studies 136
6.2.1 Pairwise selection scale 139
6.2.2 Importance and Uncertainty 142
6.2.3 Attention and Effort 143
6.3 Impact of Intuition on the decision results 143
6.4 Theoretical and implementation challenges from the users requirements 145
6.4.1 Recommendation 1: Records of solutions at different times throughout product and process development 145
6.4.2 Recommendation 2: Combine the four tools into a single software application 146
6.5 Conclusions 147
7 Conclusions 148
7.1 Introduction 148
7.2 Discussion 148
7.3 Thesis Contribution 151
7.4 Publications 151
7.5 Theoretical Contributions 152
7.5.1 Dynamic problem structuring with values and objectives 152
7.6 Conclusions 154
7.7 Future Work 155
7.7.1 Further case studies 155
7.7.2 Guidelines for method selection 155
7.7.3 Group decision-making 156
7.7.4 Customise the software framework 156
7.7.5 AHP Scales 156
7.7.6 Commercialisation 157

Bibliography 158

Appendix A 174

Appendix B 178

Appendix C 190

List of Figures

Figure 1-1 Industrial overview from 1999 to 2009 (Federsel, 2010) 1
Figure 1-2 Drug Development Time (PhRMA, 2007) 2
Figure 1-3 Stage Gate^{TM} Framework 2
Figure 1-4 Whole Process Understanding 3
Figure 1-5 Whole Process Design 4
Figure 1-6 Whole Process Design tasks, adapted from Manipura (2012) 4
Figure 1-7 Relationship between academic and industrial research 7
Figure 2-1 Pareto frontier for a two dimensional problem 12
Figure 2-2 History of Decision-Making Techniques 13
Figure 2-3 Publication history of Multi-Objective Optimisation Methods 14
Figure 2-4 Publication history of Multi-Attribute Methods 15
Figure 2-5 Publication history of Outranking Methods 16
Figure 2-6 Decision-Making Process 17
Figure 2-7 A complex adaptive system (McCarthy et al., 2006) 19
Figure 2-8 Flow chart of the ABC Algorithm (Karaboga, 2009) 30
Figure 2-9 Example reciprocal matrix in AHP 33
Figure 2-10 PROMETHEE Preference Functions (Dias, et al., 1998) 39
Figure 2-11 Example of GAIA Plane (Brans & Mareschal, 2005) 39
Figure 2-12 ORESTE Preference Structures (Bourguignon & Massart, 1994) 41
Figure 2-13 Investment Decision Tree Example (UCL, 2012) 44
Figure 2-14 Example Influence Diagram (Marks, 2004) 44
Figure 2-15 Bayesian Belief Network Example (Fenton & Neil, 1999) 45
Figure 2-16 Allais Paradox with a modified currency 49
Figure 2-17 Illustration of a value function in Prospect Theory 50
Figure 2-18 Example of a Fuzzy Set for the definition of “hot” 51
Figure 2-19 BASF Environmental Fingerprint Example (Saling, et al., 2002) 53
Figure 2-20 BASF Eco-Efficiency plot (Saling, et al., 2002) 53
Figure 3-1 The percentage of respondents who face decisions at each stage of WPD 68
Figure 3-2 Maximum time the respondents have to solve a decision problem 70
Figure 3-3 Percentage of respondents who feel comfortable using utility functions 71
Figure 3-4 Box plot of the importance of certain design features 71

Figure 4-1 Qualitative input for the MARE Method 78
Figure 4-2 A hypothetical output of the MARE methodology 79
Figure 4-3 Overview of the ChemDecide Framework 82
Figure 4-4 Decision Structure Logical Overview 84
Figure 4-5 AHP Logical Overview 86
Figure 4-6 MARE Logical Overview 89
Figure 4-7 RANK Logical Overview 90
Figure 4-8 Descending and Ascending Distillation Algorithms 93
Figure 4-9 ChemDecide Implementation Overview 95
Figure 4-10 Example Chart in the RANK module 96
Figure 5-1 AHP criteria weights for the Robinson Brothers case study 100
Figure 5-2 Final scores of the AHP analysis for the Robinson Brothers case study 101
Figure 5-3 AHP decision variables for the Robinson Brothers case study 102
Figure 5-4 MARE and RANK criteria weights for the Robinson Brothers case study 102
Figure 5-5 Final scores of the MARE analysis for the Robinson Brothers case study 103
Figure 5-6 MARE likely decision variables for the Robinson Brothers case study 104
Figure 5-7 Results of the RANK analysis for the Robinson Brothers case study... 104
Figure 5-8 RANK Credibility index for the Robinson Brothers case study 105
Figure 5-9 RANK Credibility index after removing the veto thresholds 106
Figure 5-10 Result of RANK after removing the veto thresholds 106
Figure 5-11 AHP criteria weights for the GSK case study 108
Figure 5-12 Final scores of the AHP analysis for the GSK case study 109
Figure 5-13 AHP decision variables for the GSK case study 109
Figure 5-14 MARE criteria weights for the GSK case study 110
Figure 5-15 Final scores of the MARE analysis for the GSK case study 111
Figure 5-16 MARE most likely decision variables for the GSK case study 112
Figure 5-17 RANK criteria weights for the GSK case study 112
Figure 5-18 RANK Results Chart for the GSK decision problem 113
Figure 5-19 RANK Credibility index for the GSK case study 113
Figure 5-20 Comparison of the criteria weights for the GSK case study 114
Figure 5-21 Comparison of the decision variables for the GSK case study 115

Figure 5-22 AHP criteria weights for the FFIC case study 120
Figure 5-23 Final scores of the AHP analysis for the FFIC case study 121
Figure 5-24 AHP decision variables for the FFIC case study 121
Figure 5-25 MARE criteria weights for the FFIC case study 122
Figure 5-26 Minimum/Maximum selection for c5 ('ease of operation') 122
Figure 5-27 Final scores of the MARE analysis for the FFIC case study 124
Figure 5-28 MARE likely decision variables for the FFIC case study 124
Figure 5-29 RANK criteria weights for the FFIC case study 125
Figure 5-30 Results of the RANK analysis for the FFIC case study 125
Figure 5-31 RANK Credibility index for the FFIC case study 126
Figure 5-32 Comparison of the three analyses criteria weights (FFIC) 126
Figure 5-33 Comparison of the three analyses decision variables (FFIC) 127
Figure 6-1 Results and inconsistencies in the GSK case study 137
Figure 6-2 Results and inconsistencies in the FFIC case study 138
Figure 6-3 Input of pairwise comparisons in the AHP tool 140
Figure 6-4 Dispersion of preferences in Satay's scale 140
Figure 6-5 Dispersion of preferences in balanced scales 141
Figure 7-1 Dynamic Decision Problem Structuring (Corner, et al., 2001) 153
Figure 7-2 Dynamic Decision Problem Structuring with Values and Objectives 153

List of Tables

Table 2-1 Benefits and Limitations of NPD Frameworks (McCarthy et al., 2006)... 20
Table 2-2 Comparison between AHP and ANP.. 35
Table 2-3 Benchmark study of Decision-Making Methods Groups 57
Table 3-1 Companies who responded to each questionnaire 65
Table 3-2 Handwritten decision-making methods identified from the questionnaires 66
Table 3-3 Typical stages and decisions in Whole Process Design 67
Table 3-4 Industrial Specification 74
Table 4-1 Comparison of the analysis methods in the ChemDecide Framework..... 81
Table 4-2 Consistency Values (Saaty, 1980) 87
Table 5-1 Criteria for Robinson Brothers decision problem..................................... 99
Table 5-2 Alternatives for GSK case study.. 107
Table 5-3 Criteria for GSK case study 107
Table 5-4 Comparison of the three analyses results in the form of an ordinal rank 116
Table 5-5 Sensitivity study of the RANK criteria weights 116
Table 5-6 Sensitivity study of the RANK and MARE decision variables............. 117
Table 5-7 Criteria for FFIC premix equipment selection problem 119
Table 5-8 Minimum and maximum values for criteria c1 and c2.......................... 123
Table 5-9 Four most influential criteria in AHP, MARE and RANK (FFIC) 125
Table 5-10 Comparison of the three analyses (FFIC).. 128
Table 5-11 Sensitivity of the criteria weights for the FFIC case study.................. 128
Table 5-12 Sensitivity of the decision variables for the FFIC case study.............. 129
Table 5-13 Industrial users who evaluated the framework 131
Table 6-1 Scale of the AHP Method (Saaty, 1980; Saaty & Vargas, 2012) 139
Table 7-1 AHP Scale values 157

Notation

a_{ij}	Decision variable of i^{th} alternative in respect to the j^{th} criterion
A_i	The i^{th} alternative
b_j	Criteria weights (pre-normalisation)
C_j	The j^{th} criterion
$C(A,B)$	Concordance index for alternative *A* against alternative *B*
d_j	Positive deviational variable of the j^{th} objective
$D(A,B)$	Discordance index for alternative *A* against alternative *B*
e_j	Negative deviational variable of the j^{th} objective
E	Energy
F	Feasible region in the decision space that satisfies all constraints
I	Indifferent
K	Boltzmann constant
m	Number of alternatives
n	Number of criteria
$\underline{n}$	Vector of *j* negative deviational variables
p_j	Preference threshold of the j^{th} criterion
P_i	Probability of the i^{th} choice
$\underline{p}$	Vector of *j* positive deviational variables
q_j	Indifference threshold of the j^{th} criterion
R	Incomparable
s	Intermediate value between the indifference and preference thresholds
$S(A, B)$	Credibility index for alternative *A* against alternative *B*
t_j	Numerical target level of the j^{th} objective
T	Temperature
U	Utility
v_j	Veto threshold of the j^{th} criterion
V_i	Value of the i^{th} outcome
w_j	Criteria weights (post-normalisation), where $\sum_{j=1}^{n} w_j = 1$
Z	Final rank
$Z1$	Descending distillation
$Z2$	Ascending distillation
λ	Credibility degree

Terminology

Alternative: The term is used to define an action, option, scenario or potential outcome from a feasible set among which a choice has to be made. There can either be a finite number of explicitly defined discrete alternatives or implicitly defined continuous alternatives.

Criterion: An attribute which is used to evaluate a decision problem. A criterion is either quantitative (measured on a clear defined numerical scale) or qualitative (immeasurable on a numerical scale, instead defined by subjective preferences).

Criterion Weight: The measure that reflects the relative importance of a given criterion.

Decision-Maker: The person who is responsible for solving a decision problem.

Decision Variable: A quantitative or qualitative measure of performance set by a decision-maker to evaluate an alternative with respect to a criterion.

Objective: An aim in terms of mathematical programming.

Risk: Uncertainty where alternatives can have an undesired loss.

Stakeholder: A person, group or organisation that can be affected by the outcome of a decision.

Uncertainty: The lack of certainty. A state of having limited knowledge in regards to a selection.

"If I had one wish, it is to see organizations dedicating some effort to study their own decision processes and their own mistakes, and to keep track so as to learn from those mistakes." Nobel Prize Winner, **Daniel Kahneman** (2003)

1 Thesis Introduction and Overview

1.1 Thesis Motivation

Research has shown that between 1999 and 2009, pharmaceutical sales have steadily increased (Figure 1-1). However, this has to be placed in the context that pharmaceutical development can take up to 15 years (Figure 1-2) and it is likely the sales figures in Figure 1-1 were influenced by products/processes developed prior to the start of the study. Figure 1-1 also shows that the cost of research and development (R&D) and development times (time to market) have also increased between 1999 and 2009. This occurred during a period where fewer novel drugs have been discovered. Considering over 14 million different molecular compounds have been synthesised and less than 1% (100,000) of these are on the market (Charpentier, 2007), the probability of discovering a new drug with commercial potential is very low.

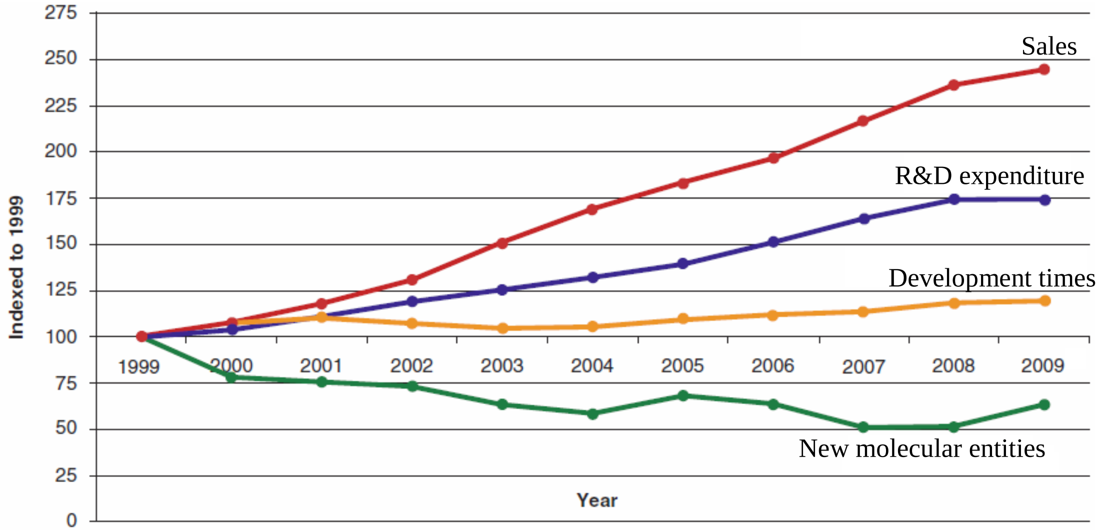


Figure 1-1 Industrial overview from 1999 to 2009 (Federsel, 2010)

The fine chemical industry is also facing challenges with Cassidy et al. (2011) stating "*instability and uncertainty bedevil the chemical industry - chiefly, in demand* *growth*". According to Diercks (2012), the recent reduction in chemical demand is a consequence of a tightened monetary policy in China and the debt crisis in Southern Europe. Cassidy et al. (2011) suggests that "*chemical companies must develop well thought out strategies and skills to deal with the changing dynamics*".

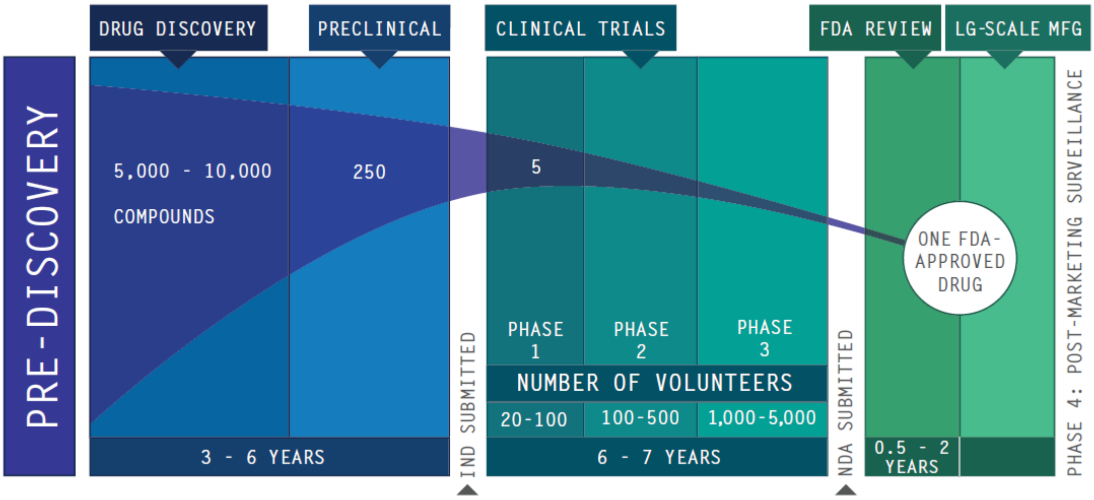


Figure 1-2 Drug Development Time (PhRMA, 2007)

One such strategy is the Stage Gate™ framework (Cooper, 2001) which divides product development into a series of consecutive stages and gates (Figure 1-3). Unlike traditional project milestones that are controlled by deadlines, gates provide greater flexibility with regards to time.

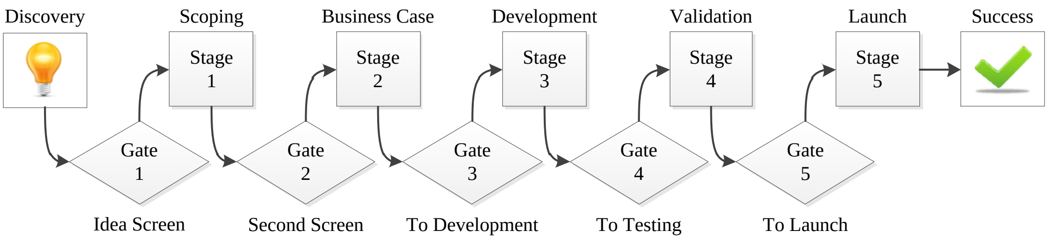


Figure 1-3 Stage Gate™ Framework

According to Cooper (2001), the advantages of the Stage Gate™ framework are early detection of failure, higher success rates, improved teamwork and reduced time to market. However, Sethi and Iqbal (2008) stated that when a gate system is rigourusly followed, the development flexibility required for product innovation is greatly reduced as companies assign project paramaters that are rigid and unchangeable when the project is approved at the initial gates. As a consequence, companies are forced to overlook changes that have occurred to business drivers such as costs, resources and time as well as factors such as health, safety and the environment.

Britest Limited, a not-for-profit organisation that correlates ideas and tools between industry and academia, identified that industry needs flexible product innovation to meet business needs. They consequently developed the concept of Whole Process Understanding (WPU) which ensures companies consider the whole process at every stage of product/process development (Figure 1-4).

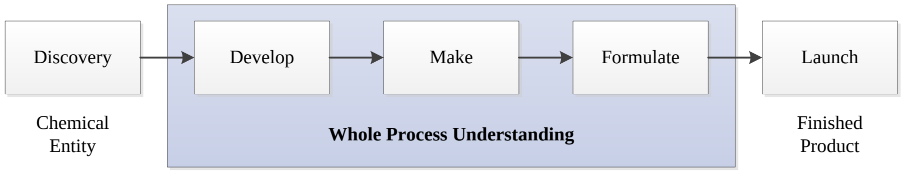


Figure 1-4 Whole Process Understanding

Between 2001 and 2012, it is estimated that industrial members of Britest Limited have saved in excess of £600 million by applying innovative tools and methodologies that utilise WPU (Britest Ltd, 2012). One such method is Whole Process Design (WPD) which considers the improvement of a whole process, from raw materials to end product, rather than the more traditional approach of enhancing a process in sequential steps. Britest acknowledged that WPD can be used to achieve rapid reactions, sustainable chemical processing and more flexible plant designs (Reay, et al., 2008). Examples of WPD include (Double, 2010):

- Determining the order of process operations.
- Optimising the stages of a multi-stage process.
- Selecting components such as reagents and solvents.
- Choosing the number of phases present in different parts of a process.
- Optimising the reaction conversion to reduce impurity formation, so that the separations become much easier.

To achieve these objectives, WPD considers process and product design simultaneously (Figure 1-5). Process design involves managing activities that produce a product while product design determines the strategic development of a product that has value (by being competitive or novel in the marketplace).

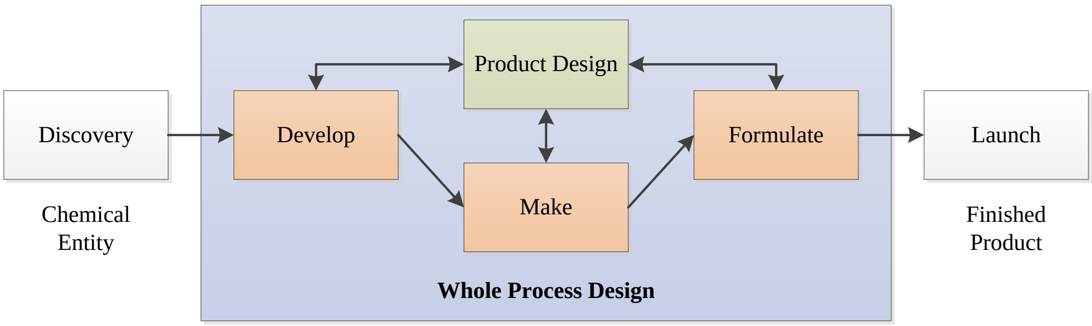


Figure 1-5 Whole Process Design

Figure 1-6 illustrates that both development functions are closely linked with some factors (in blue) already considered concurrently, such as manufacturing and quality control. However, the independent factors (in orange and green) also must be considered when implementing WPD.

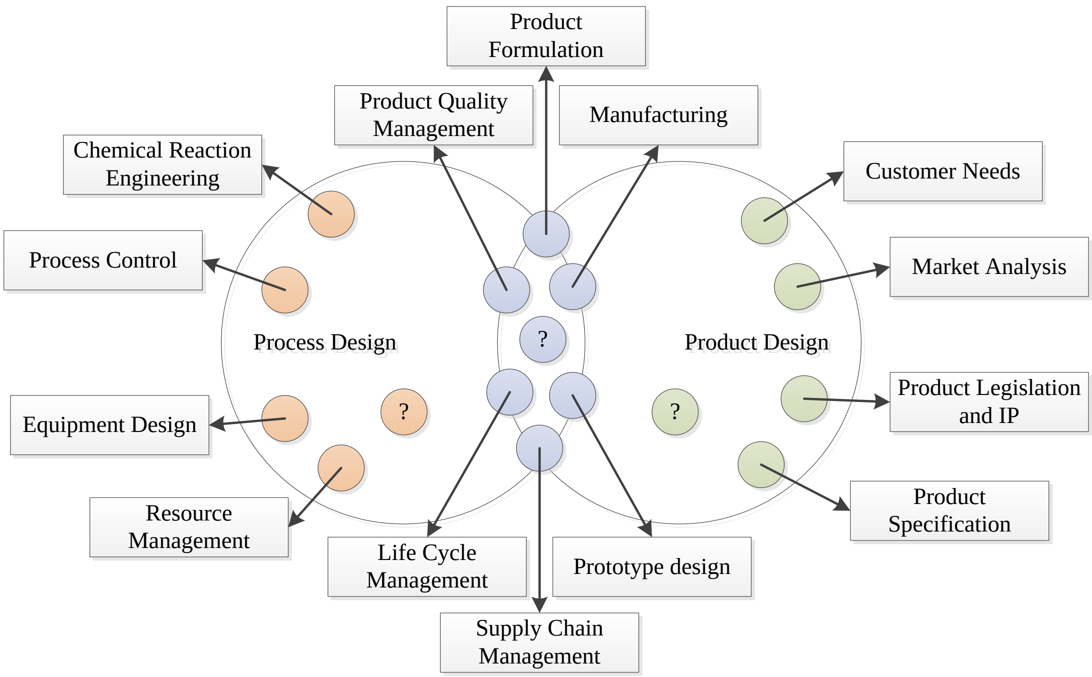


Figure 1-6 Whole Process Design tasks, adapted from Manipura (2012)

Sharratt (2011) discussed WPD in detail, explaining that there are many different decisions that must be considered when developing an effective product. These decisions impact on the product and process in multiple ways. For each decision there will be multiple criteria to consider and these will often be dissimilar or interdependent and hence represented by different measurement units. Furthermore, there will be gaps and uncertainties present in a company's knowledge and understanding about a process. This uncertainty will be more prevalent at the start of process development as less is known about the product and process.

Sharratt (2011) recognised that specialised techniques may be required to make WPD decisions effectively and that larger organisations are likely to have systems in place. However, it is unknown how effective these solutions are for highly complex problems that involve multiple criteria and uncertainty.

Considering that decision-making in industry is frequently overlooked and rarely assessed (Schrage, 2003) and that product development decisions can affect a company for up to a decade (Ng, 2004), it is essential to identify effective decision-making solutions for use during WPD.

1.2 Aims and Objectives

The primary aim of this thesis is to develop an effective decision-making solution for application during WPD. Key objectives include:

- Understanding the types of decision-making methods available in the scientific literature and the traditional methods used by the fine chemical and pharmaceutical industries.
- Identifying the industrial requirements and constraints for an effective decision-making solution.
- Understanding the different decision problems faced in the implementation of WPD.

Given that a suitable decision-making method can be developed, prototype software requires to be written that can be used to evaluate the proposed solution alongside the requirements of industry. If the solution satisfies the requirements, it will be used by Britest Limited to address challenges in the area of decision-making raised by companies in the pharmaceutical, fine chemical, mining and fuel additive sectors.

1.3 Research Questions

The overarching research question that underpins this thesis is:

RQ1: What is the most effective way to support decision-making in whole process design?

The answer to this question is dependent on a number of factors which are addressed through the literature review, interviews, questionnaires, methodological development and industrial evaluation. A series of questions thus considered include:

RQ2: Which methods in the literature are the most commonly cited/applied for solving multi-criteria decision problems? Furthermore, which of these methods are most suitable for handling uncertainty?

RQ3: Which methods in the literature have been proposed or used for decision-making in process design?

RQ4: What techniques are currently being used for decision-making in industry?

RQ5: What are the most common decisions made in WPD and in what stage of development are they considered?

RQ6: What does industry require from a decision-making framework?

Further questions will be introduced throughout the thesis as the knowledge and understanding advances.

1.4 Industrial Relationship

The work presented in this thesis has been motivated by the needs of industrial practice through a unique collaboration with Britest Limited. Britest were conscious of the potential benefits to be gained from supporting the novel and industrially significant research covered in this thesis. Accordingly, access was given to their industrial membership which included Abbott Laboratories Ltd, Pfizer Ltd, AMRI Global, Fujifilm Colorants Ltd, Procter & Gamble, GlaxoSmithKline plc, Johnson Matthey, AstraZeneca, Robinson Brothers Ltd, Infineum and Shasun. The collaboration with the industrial members allowed for the requirements of a decision-making framework to be identified and for the proposed solution to be evaluated. The advantages of working with the Britest members was that they are well-acquainted with the concepts of WPD, hence they were in a position to provide insight and to critically evaluate a decision-making solution for WPD. Figure 1-7 summaries the relationship between the industrial and academic research encapsulated with this thesis.

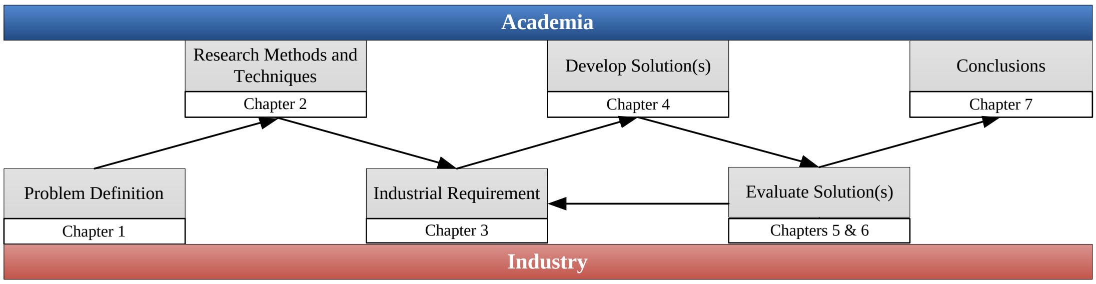


Figure 1-7 Relationship between academic and industrial research

1.5 Thesis Structure

Chapter 2, methods and techniques, critically reviews literature pertaining to existing decision-making methodologies that are applied in the fields of operational research, engineering, management science and decision support systems. In addition, human personality characteristics are considered by examining the psychological aspects of decision-making in relation to behavioural sciences. The chapter concludes with a discussion of the key publications that demonstrate or discuss decision-making in the process industry.

Chapter 3 identifies the industrial requirements for developing a decision-making framework for use during Whole Process Design (WPD). Following a discussion with industrial decision-makers, two questionnaires are circulated and the findings are evaluated with the aim of identifying the key characteristics of a decision-making methodology.

The Multi-Attribute Range Evaluations (MARE) method is introduced in Chapter 4. The technique is described in detail along with an evaluation strategy which consists of developing a framework that utilises the MARE method along with two other decision analysis tools. The framework termed ChemDecide also includes a problem structuring software that is referred to as Decision Structure.

Chapter 5 evaluates the ChemDecide framework through three industrial WPD decision-making case studies. The first case study focuses on a chemical route selection problem provided by Robinson Brothers Ltd. The second is based around the selection of degassing reagents in conjunction with GlaxoSmithKline (GSK). The third is undertaken with Fujifilm Imaging Colorants Ltd (FFIC) and aims to select the best equipment to mix a substance at the early stages of process development.

Chapter 6 presents a discussion based on the findings of the three case studies. Inconsistencies in the case studies are identified and assessed, the role of intuition is examined and future requirements are evaluated.

Chapter 7 concludes the thesis by discussing the initial research question, summarising the conclusions and presenting further work.

"The world moves into the future as a result of decisions, not as a result of plans. Plans are significant only insofar as they affect decisions... if planning is not part of a decision making process, it is a bag of wind, a piece of paper, and worthless diagrams." **Kenneth E. Boulding** (1974)

2 Methods and Techniques

2.1 Introduction

This chapter aims to answer the following two research questions by critically reviewing the academic literature:

RQ2: Which methods in the literature are the most commonly cited/applied for solving multi-criteria decision problems? Furthermore, which of these methods are most suitable for handling uncertainty?

RQ3: Which methods in the literature have been proposed or used for decision-making in process design?

The first two sections aim to address RQ2 by reviewing the most commonly applied methods for Multi-Criteria Decision Analysis (MCDA). As MCDA is inherently linked to cognitive psychology, economics and various other disciplines, the third section reviews the implications of using these methods from a behavioural perspective. The section discusses how individuals and groups construct judgements and form choices whilst examining rational choice, irrational behaviour and uncertainty. The final section addresses RQ3 by reviewing the use of decision-making methods in Whole Process Design (WPD).

2.2 Decision-Making Techniques

This section starts by discussing the history of decision-making methods and then introduces the theories behind a range of modern day decision-making techniques. The second section discusses the decision-making process, from identifying a decision problem through to presenting a solution. The remaining sections introduce and evaluate the most commonly applied decision-making methodologies discussed in the academic literature.

2.2.1 History of Decision-Making Techniques

Decision-making has been discussed by many great ancient philosophers including Plato, Aristotle and Thomas Aquinas (Figueira, et al., 2005). However the first documented approach which led to the modelling of a decision problem originated from a discussion between Blaise Pascal and Pierre de Fermat in 1654. The discussion concerned a game of chance with two players who have equal opportunity to win a sum of money. The players contribute equal fees to play the game and agree to the winning terms. However, the mathematicians identified a problem which arises when considering the fair division of money if the players need to end the game early, before the winning terms have been met. Both Pascal and Fermat (1654-1660) independently devised a solution which was based on the same fundamental principle. They agreed that the division had to be proportional to each player's chance of winning. This formed the basis of expected value theory which considers the probability of a win multiplied by its value:

$$EV = \sum_{i=1}^{m} V_i * P_i \qquad \textbf{2-1}$$

where EV is the expected value, i denotes each of the different consequences, P_i is the probability of the i^{th} choice and V_i is the value of the i^{th} outcome.

However, it was identified that human behaviour can violate expected value theory as the theory infers a rational decision-maker will always desire the maximum expected value. Nicolas Bernoulli devised a problem to challenge expected value theory which is now commonly called the St. Petersburg paradox (Bernoulli & de Montmort, 1713). The paradox considers a game of chance where a coin with two sides, *A* and *B*, is tossed repeatedly until side *B* appears. A player pays a fixed fee to enter and receives a cash prize that is doubled every time side *A* appears. The fundamental problem associated with this paradox is assigning a fair fee to play the game. When considering this problem using expected value theory, the winning sum always converges to infinity. Therefore, by following expected value theory, a rational player should enter the game paying any finite amount as the outcome will be higher than any fixed fee. However, in reality, every rational person has a logical threshold which they consider a fair entry fee due to limitations in personal wealth and tolerance to risk. Thus, personal value of an outcome should be considered differently from its objective monetary value. Bearing this in mind, Daniel Bernoulli, Nicolas Bernoulli's cousin, presented a solution to the St Petersburg paradox in 1738. The solution (Bernoulli, 1738) was to use a logarithmic utility function to modify the expected value depending on the player's wealth. This was the first systematic occurrence of expected utility theory (which is sometimes referred to as subjective probability). Expected utility theory in its modern form refers to a cardinal utility function which assigns a value of desirability to each alternative. This approach, as illustrated in equation 2-2, was derived largely from two game theorists; John Von Neumann and Oskar Morgenstern (Von Neumann & Morgenstern, 1947).

$$EU = \sum_{i=1}^{m} U(a)_i * P_i \qquad \textbf{2-2}$$

where *EU* denotes the expected utility, *i* defines the different consequences, P_i is the probability of the i^{th} choice and $U(a)_i$ is the decision-maker's utility of the i^{th} outcome.

Expected utility theory has generally been accepted as the standard method to model rational choice. Nevertheless, there are a number of problems presented by Kahneman and Tversky (1979) which violate the axioms of expected utility. They proposed the use of non-expected utility theory which is discussed further in section 2.3.3.

Constructing a utility function generally requires the consideration of two or more criteria. These criteria are often interdependent and/or conflict with one another. This concept started the discussions between Edgeworth (1881) and Pareto (1906) with regards to the analysis of a multi-criteria problem. Edgeworth proposed the term optimum to indicate the ideal point between a number of trade-offs for a multi-criteria problem. This point is referred to as the Edgeworth-Pareto optimal or more commonly, the Pareto optimal (as Pareto generalised the theory). A point is said to be Pareto optimal if there exists no feasible arrangement of decision variables that would decrease some criterion without causing an associated increase in at least one other criterion. Normally there is not a single Pareto optimal point but rather a set of solutions termed a Pareto optimal set. If the Pareto optimal set is drawn in a two or three dimensional objective space, the formulation is referred to as the Pareto frontier (Figure 2-1). A Pareto frontier is often used to illustrate a feasible set of alternatives which a decision-maker can evaluate rather than considering every possible solution.

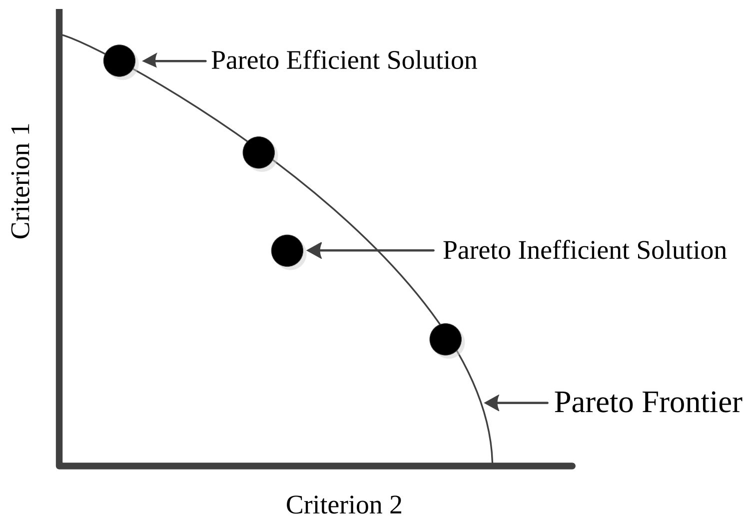


Figure 2-1 Pareto frontier for a two dimensional problem

Over the past fifty years a number of different decision-making techniques have emerged to sort, rank or quantify alternatives based upon Pareto optimal selection. These methods can be separated into three categories, Multi-Objective Optimisation (MOO), Multi-Attribute (MA) and Outranking methods. MOO algorithms are based on maximising or minimising certain objective functions to identify the optimum values that satisfy a number of requirements. Generally there is no attempt to capture the decision-maker's utility functions mathematically in this approach. Instead MOO algorithms use implicit information about the decision-maker's preferences to steer the algorithm's search. Typically MOO methods are used when there are a large or infinite number of feasible solutions. MA methods and outranking approaches on the other hand are generally used in discrete decision problems with a small to moderate number of feasible solutions. Consequently, these methods are better suited to handling uncertainty (Wallenius, et al., 2008) and are computationally less intensive than MOO methods. Outranking approaches differ from MA methods as they accept that one alternative may have a degree of dominance over another. This is interpreted by a pairwise outranking relationship formed by aggregating each possible pair of alternatives. When this data is combined, a partial or complete ordinal ranking is determined. MA methods, in contrast, aggregate every criterion into a function which is maximised. Although MA and outranking approaches are often considered similar, MA methods produce numerical outputs while outranking methods produce an ordinal rank to infer the decision-maker's preferences.

All three families of MCDA methods comprise of a number of approaches that have their own unique advantages and limitations. Figure 2-2 presents these approaches along with their respective interactions and relationships to previously reported theories and methodologies. The theories and methodologies are arranged in order of publication year, starting with expected value theory at the top to the most modern approaches at the bottom.

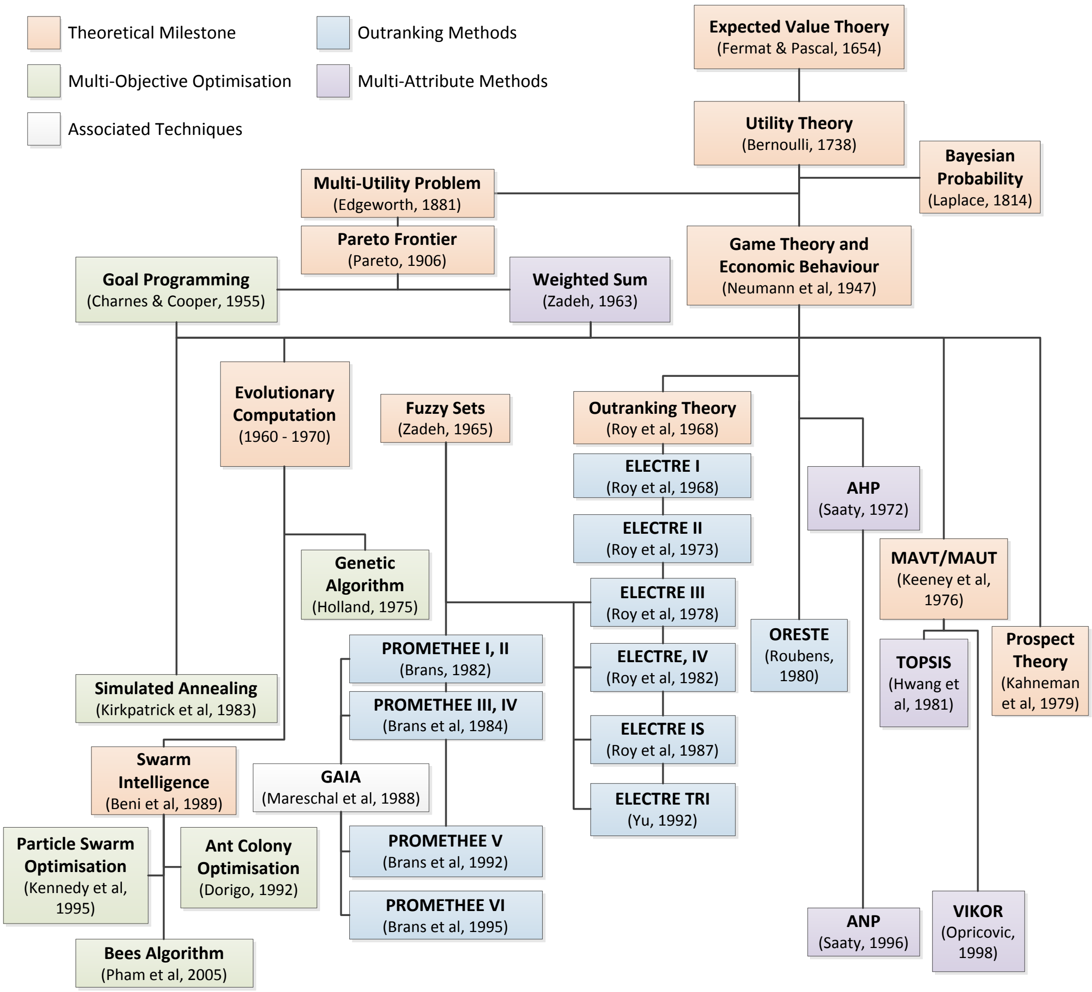
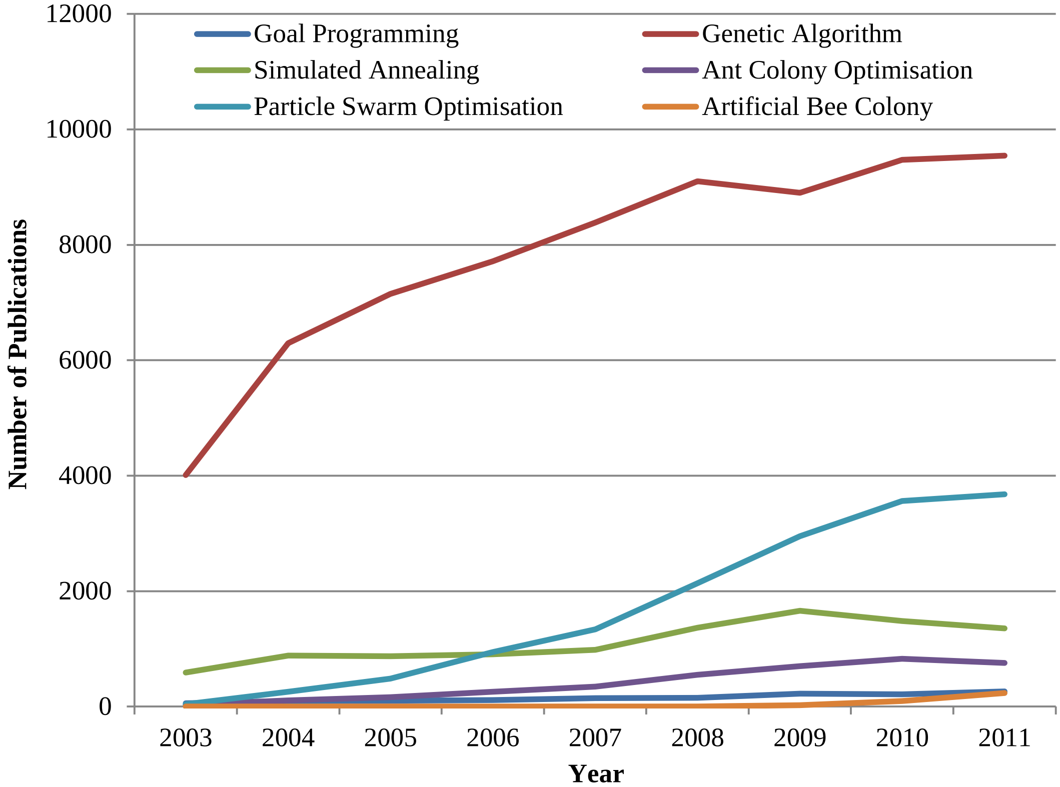


Figure 2-2 History of Decision-Making Techniques

Figure 2-3 shows the number of publications relating to the methods within the field of MOO between 2003 and 2011. It can be observed that, Genetic Algorithms have received the largest level of interest with a steady increase from 2003 to 2011. Particle swarm optimisation has also shown a significant rise in publications. In contrast, goal programming, simulated annealing, ant colony systems and artificial bee colony have shown minor but steady growth.



Based upon a keyword bibliometric study using the SciVerse database.

Data acquired 31/07/2012

Search Terms

Goal Programming: "Goal Programming"

Genetic Algorithm: "Genetic Algorithm"

Simulated Annealing: "Simulated Annealing"

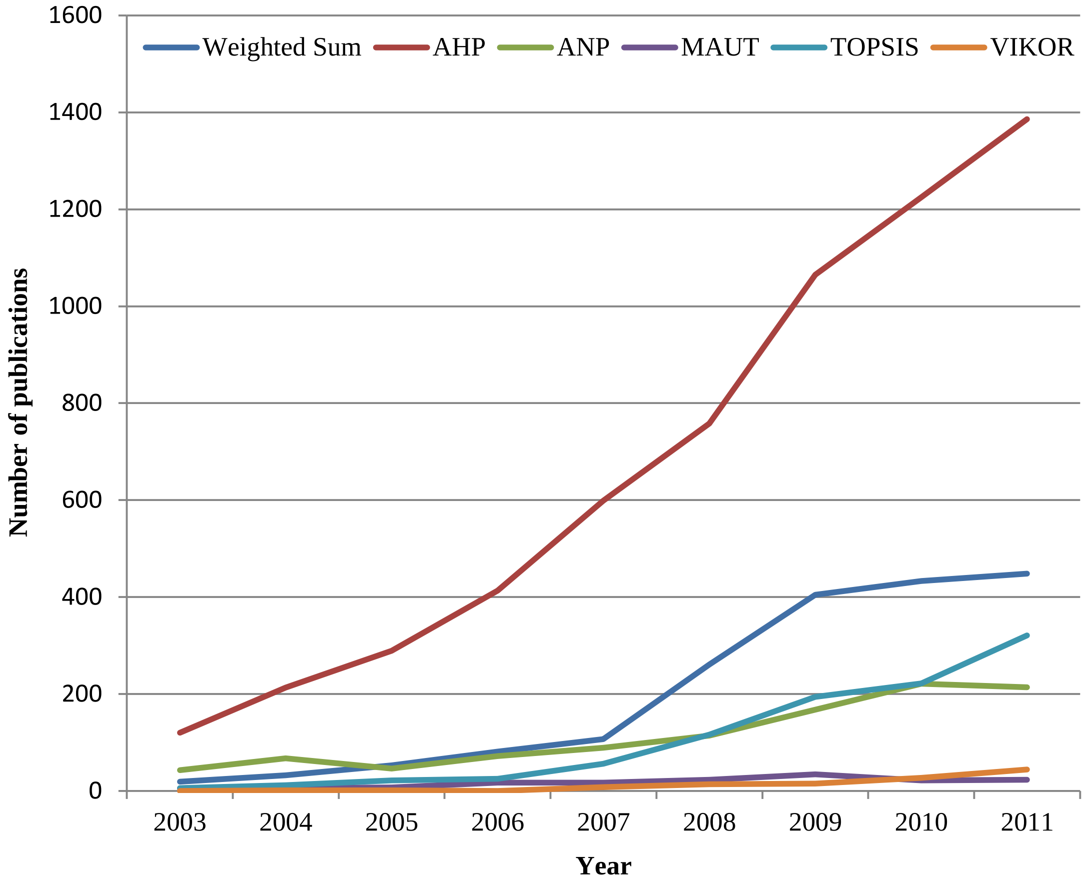
Ant Colony Optimisation: "Ant Colony Optimisation" OR "Ant Colony Optimization"

Particle Swarm Optimisation: "Particle Swarm Optimisation" OR "Particle Swarm Optimization"

Artificial Bee Colony: "Artificial Bee Colony"

Figure 2-3 Publication history of Multi-Objective Optimisation Methods

Figure 2-4 shows the number of publications relating to MA methods between 2003 and 2011. It is evident that the Analytic Hierarchy Process (AHP) has received the greatest growth in interest during the last decade. Huang et al (2011) who also identified a significant growth in AHP related publications suggests "*the wide use of AHP may be related to the availability of user-friendly and commercially supported software packages and enthusiastic and engaged user groups*". The Weighted Sum Method (WSM), Analytic Network Process (ANP) and Technique for Order Preference by Similarity to Ideal Solutions (TOPSIS) methods have also seen increased interest since 2007. The interest in Multi-Attribute Utility Theory (MAUT) and VIKOR has been relatively stable during this period.



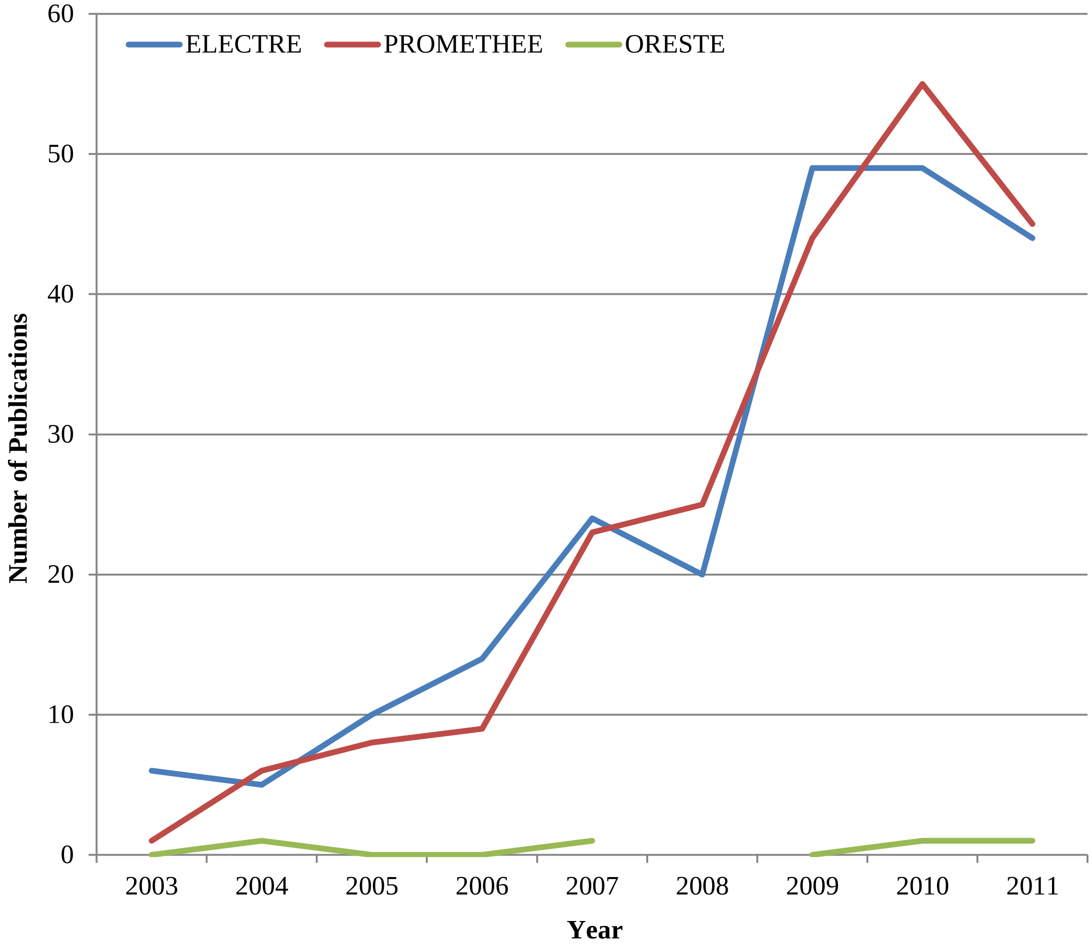
Based upon a keyword bibliometric study using the SciVerse database.
Data acquired 31/07/2012

Search Terms

Weighted Sum: "Weighted Sum"
AHP: "Analytic Hierarchy Process" OR "AHP"
ANP: "Analytic Network Process" OR "ANP"
MAUT: "MAUT" OR "multi attribute utility theory" OR "multi-attribute utility theory"
TOPSIS: "TOPSIS"
VIKOR: "VIKOR"

Figure 2-4 Publication history of Multi-Attribute Methods

Figure 2-5 shows the number of publications relating to outranking methods between 2003 and 2011. Outranking methods, which are generally regarded as the French or European school of thought, have recieved less acadmic interest. Huang et al (2011) suggest that the European methods have a "*stronger theoretical school and a varied MCDA culture*" which could account for the lesser interest. Another cause could be due to the language barrier, as the bulk of early outranking literature is written solely in the French language. It has only been in recent years that this literature has been translated and discussed by English speaking readers. Although the publication scale of the outranking approaches is insignificant in contrast to MOO and MA techniques, the ELECTRE and PROMETHEE methods have shown a steady growth of interest.



Based upon a keyword bibliometric study using the SciVerse database. **Data acquired 31/07/2012**	**Search Terms** ELECTRE: "ELECTRE" PROMETHEE: "PROMETHEE" ORESTE: "ORESTE"

Figure 2-5 Publication history of Outranking Methods

2.2.2 Decision-Making Processes

This section is divided into two parts. The first introduces the phases of a decision-making process whilst the second discusses the stages of New Product Development (NPD).

2.2.2.1 Decision-Making Process

Decision-making literature has focused primarily on developing methods or applying pre-existing approaches to particular problems with little emphasis on the decision-making process (Belton & Stewart, 2010). However, Belton & Stewart (2010) and Franco & Montibeller (2009) agree that the decision-making process consists of a number of phases (Figure 2-6) including problem structuring, decision analysis and post analysis.

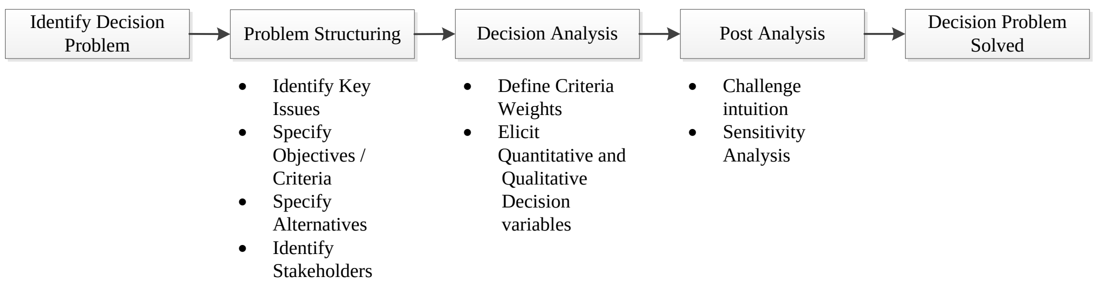


Figure 2-6 Decision-Making Process, adapted from Belton & Stewart (2010); Franco & Montibeller (2009)

Franco and Montibeller (2009) consider the problem structuring phase as the most neglected aspect of the decision-making process. They believe this is due to a common assumption that forming a well structured problem is a somewhat trivial task. Many decision-makers want to progress to the decision analysis quickly without considering that an erroneous decision model will most likely provide inaccurate results. However, problem structuring is a complex task that requires the decision-maker to organise their thoughts with the aim of identifying objectives, criteria, alternatives, stakeholders and other key information about the problem. Belton & Stewart (2010) proposed the use of the acronmym "CAUSE" (Criteria, Alternatives, Uncertainties, Stakeholders and External/Environmental) to promote the key elements of the problem structuring phase. The problem structuring process is generally regarded as a cognitive task; however there are a few approaches that aim to systematically guide the identification of effective criteria and alternatives. Keeney (1992) introduced the concept of value focused thinking which looks at identifying objectives and criteria to generate and evaluate alternatives. It was proposed after noting that the majority of decision-makers focus on establishing alternatives first rather than criteria (alterntive focused thinking). Keeney (1992) believed that "*better alternatives*" can be selected once the criteria are established.

More recently, Corner, et al. (2001) proposed a different solution as they believed problem structring is an iterative process. Their method, dynamic decision problem structuring, cycles between value focused thinking and alternative focused thinking. The idea is that the consideration of criteria prompts creative thinking about the alternatives which in turn generates new criteria, and so on. Belton and Stewart (2010) stated "*the iterative process* [of dynamic decision problem structuring] *encourages decision makers to reflect on and learn about their values and the problem context*". Nevertheless, Franco & Montibeller (2009) believe that there is still need for further work in this field. They suggest that structed tools are required for problem structuring which consider the psychological asepects (e.g. how to instigate creativity) and group dynamics (e.g. how to identify and display complex scenarios to a group of decision-makers).

The next phase of the decision-making process is the analysis of the problem. This involves defining decision variables and criterion weights that represent the decision-maker's preferences. The ways in which these values are integrated into the algorithm depends on the methodology selected. The various methodologies available are discussed in detail in the subsequent sections.

The final phase of the decision-making process is a post analysis study that challenges the results of the analysis. This is an important stage and allows a decision-maker to challenge their intuition and to check for any inaccuracies.

2.2.2.2 Stages of New Product Development

A number of frameworks exist that can be utilised for New Product Development (NPD) in engineering management. A popular framework that is widely cited throughout engineering literature is the Stage Gate framework which was discussed in section 1.1. The Stage Gate framework (Cooper, 2001) is considered as a linear NPD process as the various stages are completed in succession (Figure 1-3). A linear system is well-structured, predicable and can help organise and comprehend the complexity of a NPD process. However, a linear framework is inflexible and as such means innovation is constrained (section 1.1).

Other NPD processes known as recursive and chaotic frameworks overcome the limitations of inflexibility with linear frameworks. Recursive frameworks utilise feed-back and feed-forward loops to represent the dynamic and fluid nature of an innovative process. Such a framework allows for NPD stages to overlap and suggests that the process is less clear and rigid than a linear framework. A chaotic framework expands on this idea by depicting NPD processes with "*random-like and nonlinear behaviour*" (McCarthy et al., 2006). Chaotic frameworks are unpredictable, unstructured and disorganised at the initial stages of NPD with the final stages being relatively more ordered.

McCarthy et al. (2006) stated that each individual framework "*provides valuable insights and understanding about the behaviour and structure of NPD processes*". However, they proposed that a collective system that can "*switch or toggle between behaviours that range from linear to chaotic*" would have more value than an individual framework. They proposed a collective system termed Complex Adaptive System (CAS) which "*is somewhere between a linear and chaotic system*" (Figure 2-7**).**

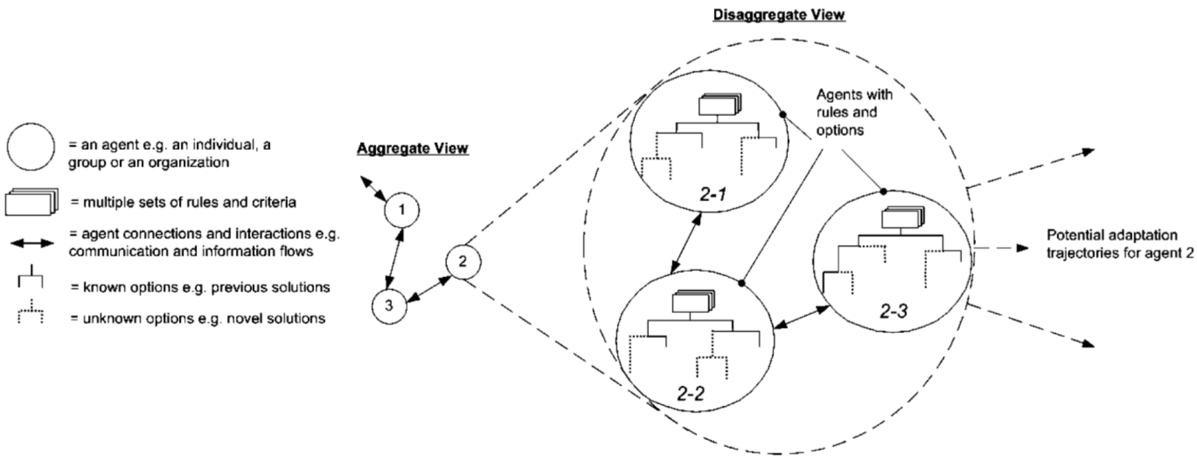


Figure 2-7 A complex adaptive system (McCarthy et al., 2006)

Figure 2-7 shows that a CAS system contains a number of partially connected agents (individuals, groups or organisations) whose interactions overlap NPD stages and decision levels. The aggregate view depicts agents as organised and structured while the disaggregate view illustrates that a single agent is composed of known and unknown options that portray nonlinearity and unpredictability. A description along with the advantages and limitations of each of the four frameworks are presented in Table 2-1.

Table 2-1 Benefits and Limitations of NPD Frameworks (McCarthy et al., 2006)

NPD	Description	Benefits	Limitations
Linear	A process with relatively fixed, discrete and sequential stages. The connections, flows, and outcomes of the process are comparatively deterministic.	Provides a simple and effective representation of the structural logic and flows. Suited to incremental innovation activity with relatively reliable market push or strong market pull forces.	Does not consider the dynamic behaviours and relationships associated with agency, freedom, and resulting innovations.
Recursive	A process with concurrent and multiple feedback loops between stages that generate iterative behaviour and outcomes that are more difficult to predict.	Represents the dynamic and fluid nature of the process. Suited to more radical innovations with push–pull market force combinations.	Assumes similar behaviour across the whole process and does not represent the structural and behavioural instabilities of the process.
Chaotic	A process where the linkages and flows are greater during the initial stages, resulting in different degrees of feedback across the process. The initial stages exhibit chaotic dynamics and outcomes that appear to be random and unpredictable, whereas the latter stages are relatively stable and certain.	Recognises different system behaviours across the process and acknowledges the effects of highly cumulative causation. Suited to the search and exploration aspects of very radical innovations or really new products.	Focuses on differences between the stages and presupposes that the overall process configuration is fixed (i.e., does not consider process adaptability).
Complex Adaptive System	A process with partially connected agents whose interactions cross stages and decision levels. Collectively they are able to produce a process dynamic between order and chaos, which results in process adaptability and the potential to generate different behaviours and innovation outcomes	Assumes that overall process configurations and behaviours are malleable. They can be internally changed to match push or pull market forces and innovation expectations that range from incremental to very radical.	Semantic confusion concerning the terms complex and complexity. Challenges in framing and measuring the process constructs coupled with the misconception that process outcomes are random and therefore unpredictable.

One form of CAS is Whole Process Design (WPD) which combines linear, recursive and chaotic processes. As shown in Figure 1-5, the initial and final stages are linear with the intermediate stages representing a combination of recursive (linkages and flows between the stages) and chaotic (the consideration of multiple known and unknown factors within all stages) processes.

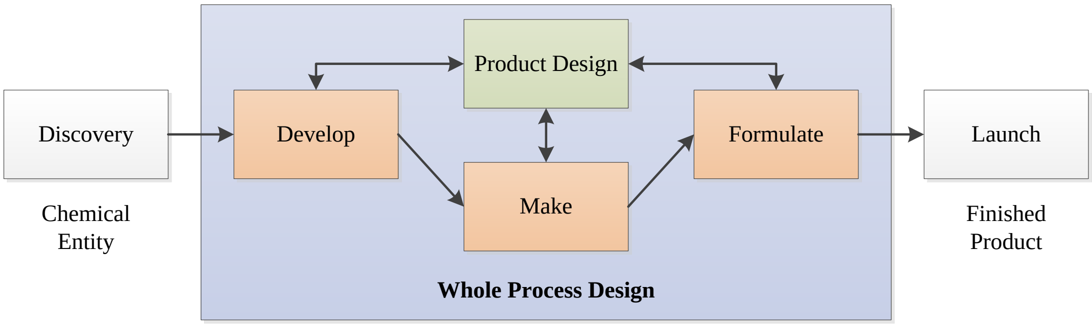


Figure 1-5 Whole Process Design

As discussed in section 1.1, WPD can be used to achieve rapid reactions, sustainable chemical processing and more flexible plant designs. The WPD framework has already been successfully adopted by the industrial members of Britest and is considered "*as a clear and useful concept within the design of low tonnage chemicals processes*" (Sharratt, 2011). However by adopting WPD, decision-making becomes more challenging as multiple factors must be considered throughout NPD. As a consequence, identifying the most effective way to support decision-making throughout WPD is the primary goal of this thesis.

2.2.3 Multi-Objective Optimisation

Multi-objective optimisation (MOO) methods are mathematical algorithms that search for values of decision variables. They aim to provide the optimum set of values for more than one objective function. Each additional objective function increases the complexity of the search space with the problem dimensionality increasing accordingly. For example, a problem with three objectives would be considered as a three dimensional problem. Multi-objective problems can be solved using an exhaustive search that checks every possible combination of decision variables. However, due to the size of the search space for even a simple multi-objective problem, the time required to conduct the search is extensive and impractical in the majority of cases. As a result of these challenges, MOO methods have received much academic interest in recent years.

Decision problems almost always contain multiple objectives that conflict with one another. For example, minimising the cost of production while maximising profit or minimising a product's weight while maximising its tensile strength. For these types of problems there will be a number of ideal solutions present in the n-dimensional search space. Furthermore, decision problems characteristically contain discrete decision variables. Optimisation problems incorporating such variables are defined as combinatorial problems and require MOO algorithms that deal with complex search spaces (Garey & Johnson, 1979). The following section presents and evaluates a number of key techniques reported in the literature that can be used to solve multi-objective combinatorial optimisation problems.

2.2.3.1 Unclassified Algorithms

a. Goal Programming

Goal programming was introduced by Charnes et al. (1955). The method is regarded as an adaptation of linear programming (Jones & Tamiz, 2010) and is commonly referred to as multi-objective linear programming. A clearer definition of goal programming was provided in the book by Charnes & Cooper (1961). Since publication, there has been a small but steady increase of academic interest surrounding the method.

In goal programming the objective or goal is defined by the term functional. Algebraically a functional can be modelled as:

$$f_j(\underline{x}) = t_j + d_j - e_j \qquad \textbf{2-3}$$

where t_j denotes the numerical target level of the j^{th} objective (set by the decision-maker), d_j is the positive deviational variable of the j^{th} objective and e_j is the negative deviational variable of the j^{th} objective.

A positive deviational variable represents the position by which the target level is over achieved. A negative deviational variable represents the level by which the target is under achieved. For example, a goal involving profit would require any negative deviation below the goal level to be penalised. An achievement function is then used to optimise the deviational variables to identify the best set of goals. The generic goal programming achievement function is presented in equation 2-4:

$$\begin{aligned} & Min\ a = h\,(\underline{n}\,, \underline{p}\,) \\ & \text{Subject to} \quad f_j(\underline{x}) + e_j - d_j = t_j \qquad j = 1, \dots, n \\ & \qquad\qquad\quad\ \underline{x} \in F \\ & \qquad\qquad\quad\ e_{j,} d_j \geq 0 \qquad j = 1, \dots, n \end{aligned} \qquad \textbf{2-4}$$

where $\underline{n}$ denotes the vector of j negative deviational variables, $\underline{p}$ denotes the vector of j positive deviational variables. F is the feasible region in the decision space that satisfies all constraints.

There are a number of other commonly used variations of goal programming including weighted goal programming, lexicographic goal programming and fuzzy goal programming which all have different achievement functions. According to Romero (2004), 21% of all goal programming applications use the weighted algorithm and 65% use lexicographic approach.

Weighted goal programming, also known as Archimedean goal programming, allows the decision-maker to attach weights of importance to each objective and minimise the sum of negative deviational variables. The standard approach is often criticised for its inability to handle criteria weights hence the popularity of weighted goal programming as it can overcome this limitation. However, a disadvantage of weighted goal programming is its inability to handle different measurement units. Tamiz et al. (1995) proposed a number of normalisation techniques to address this but there are few examples of these normalisation procedures being applied in practice. Lexicographic goal programming works differently by allowing the decision-maker to select a priority level (a rank) for each goal.

Tamiz et al. (1998) suggests the best modelling practice for most real-life problems is not to rely on one single goal programming variant but instead to use several variants of goal programming.

Goal programming can handle a large number of decision variables, objectives and constraints. However, the algorithm is sometimes incapable of finding solutions that are Pareto efficient, hence Tamiz et al. (1999) proposed a modification using integer goal programming analysis tools to ensure the achievable solutions are Pareto efficient. However, this modification adds another layer of complexity to the goal programming technique and consequently is often ignored by decision analysis practitioners.

Jones and Tamiz (2010) stated that goal programming can be "*a valuable aid*" for deicison-making in health care and portfolio selection.

b. Simulated Annealing

Simulated Annealing (SA) shares similarities with evolutionary optimisation (see section 2.2.3.2) but is not considered a direct form of the technique. The method was introduced by Kirkpatrick et al. (1983) and since the initial publication, interest has grown steadily. The method is stochastic in nature as it supports random search deviations, thereby theoretically escaping entrapment within local optima. The SA algorithm mimics the cooling of metallic solids from the liquid phase to increase the volume of crystals thereby reducing the number of defects. The initial heat applied to the material forces its atoms to freely move in random directions. As the cooling process occurs, the atom's energy will slowly decrease resulting in the discovery of a new formation. This is modelled by defining a probability *P*, using Gibbs law:

$$P = e^{\frac{E}{kT}} \qquad \textbf{2-5}$$

where *E* denotes energy, *k* is the Boltzmann constant and *T* is temperature.

Gibbs law shows the probability of the formation change is directly related to the temperature and the energy of the system. This is mimicked in SA by replacing the energy function with an objective function made up of decision variables:

$$P = \frac{-(f(y) - f(x))}{e^{kT}} \qquad \textbf{2-6}$$

where *f(y)-f(x)* is the difference between the new and old objective functions.

The general procedure of SA is as follows:

1. Define the cooling schedule (starting temperature, final temperature, temperature decrement and iterations at each temperature), objective function and initial starting point. Set frozen as false.
2. While frozen is false:
    a. Randomly generate a neighbourhood point.

    b. Calculate the energy (objective function) of the new solution.
    c. If the energy lowers, accept the new neighbourhood point.
    Else,
        i. Calculate probability of acceptance (equation 2-6).
        ii. If within probability, accept the new neighbourhood point.
    d. If frozen, set frozen as true.
3. Return low energy solution.

One major drawback of SA is that the computational time required to solve a problem can be proportional to its magnitude. For certain large and complex problems, SA may require a similar number of iterations to an exhaustive search.
As a result of this, Triki, et al. (2005) believes SA lacks practical application. Furthermore, SA requires considerable understanding to gain meaningful results. In particular, it is problematic to select a suitable cooling schedule which will accurately reflect the problem's search space. Often the cooling schedule is empirically adjusted during the algorithm's evaluation. This means the algorithm is only practically applicable by practitioners who have an in depth knowledge and understanding of the algorithm.
For SA to be more widely accepted, there is a need for real world case studies to be reported in the literature. These may provide the knowledge required to develop a dynamic cooling schedule that adapts to a multitude of problems.

2.2.3.2 Evolutionary Algorithms

Evolutionary optimisation replicates the concept of Darwinian selection computationally to identify the fittest or optimum solution. Branke et al. (2008) identified four researchers who established evolutionary optimisation between 1965-1975: Schwefel (1974) and Rechenberg (1971) developed evolutionary strategies, Fogel et al. (1966) created evolutionary programming and Holland (1975) established genetic algorithms.

a. Genetic Algorithm

The genetic algorithm (GA) is by far the most popular MOO algorithm within the field of evolutionary computing. It works in a similar manner to all evolutionary optimisation algorithms, by forming a population of solutions. This concept has a number of advantages for complex multi-objective problems as it can explore several parts of the search space simultaneously. The difference between GA and other evolutionary based algorithms is that GA is founded on the principle of genetics. Each solution in the population is represented by a chromosome. These chromosomes are altered throughout every generation (computer iteration) until a suitable solution is found.

The general procedure of a GA is as follows:

1. Define an end condition (time or number of iterations).
2. Generate a random population of chromosomes.
3. Evaluate fitness of each chromosome in the population.
4. Create a new population by repeating the following steps until a new population is complete:
   a. Select two parent chromosomes from the population according to their fitness.
   b. Crossover the parents to form a new offspring.
   c. Randomly mutate the offspring.
   d. Place the offspring into the population.
5. Evaluate fitness of each chromosome in the population.
6. If the end condition is met, return the best solution in the current population.

The crossover (4b) and mutation (4c) stages of the procedure are the main genetic operators. There are a number of techniques including permutation encoding, value encoding and tree encoding which handle the crossover stage separately. However, the most common method is binary encoding which selects a random cut off point and forms a new offspring by merging one side of the cut point of parent A to the other side of the cut point of parent B (for example, A:10001|011 and B:01101|110 produces 10001110). Sometimes multiple cut points are used to ensure the greatest amount of variation. The mutation stage consists of a small alteration to the new offspring (for example: 10001110 mutates to 10101110). The probability of this occurring to each individual bit of the chromosome is set by the decision-maker. Generally this value is fixed to less than 0.1. The level of the mutation probability denotes the stochastic nature of the algorithm.

The GA is known for its ability to find suitable search regions rapidly. However, the algorithm is not effective in terms of rapidly locating the local optimum within a suitable region. This is partly because the algorithm's population size is considered infinite when in practice the population size is finite (El-Mihoub, et al., 2006). Much work in the last decade has gone into developing hybrid or memetic GAs which can provide improved local search functions. This is discussed further in section 2.2.3.4.

2.2.3.3 Swarm Algorithms

Swarm intelligence was established by Beni and Wang (1989) for the application of artificial intelligence to cellular robotic systems. Swarm systems, similar to evolutionary optimisation, use populations of solutions to explore the local and global search spaces. The difference between them is that instead of mimicking Darwinian selection; swarm systems imitate colonies of insects or animals to gain collective intelligence.

a. Ant Colony Optimisation

Ant Colony Optimisation (ACO) was derived from the ant system which was conceptualised by Dorigo (1992) during his doctoral research. ACO is a class of swarm optimisation based on the movement of ants seeking a path between food and their colony. Ants initially wonder in random directions, avoiding obstacles, until they locate a food source. When a food source is found, the ants return to their colony releasing pheromones. Other ants that locate this pheromone trail follow it to the food source. Pheromone trails evaporate over time making shorter paths more attractive to the ants as they last longer and hence can be used more frequently. This process eventually results in the determination of the shortest path between the food source and the colony. In algorithmic terms, the artificial ants are a population of solutions that work in parallel to find an optimal solution. The algorithm functions as follows:

1. Define an end condition (time or number of iterations).
2. Define nodes (states), the attractiveness (artificial pheromones) between every node and the number of ants (population size).
3. Randomly assign a node to each ant as a starting position.
4. While end condition has not been met:

   a. Move every ant to their next node using a probability function that considers the attractiveness of each ant's connecting nodes.
   b. Update attractiveness between every node.
   c. If an ant's solution is shorter (better) than the current best solution, save new solution as best solution.
5. Return the best solution.

Gutjahr (2003) considers ACO particularly promising for three reasons:

- The algorithm uses memory (via pheromone trails), similarly to evolutionary and other swarm algorithms but different from SA and goal programming.
- Problems with a highly constrained solution space can be encoded in a natural way.
- Knowledge that is specific to the problem (problem-specific heuristics) can be used to improve the performance of the optimisation.

Gutjahr (2003) stated that the last two points give ACO a competitive advantage in addressing highly contrained combinatorial optimisation problems. Blum (2005) reviewed a number of applications of ACO, including data mining, timetabling, scheduling, vehicle routing and bioinformatics problems. Although he found many successful examples, he recommended utilising ACO with other algorithms as a hybrid search (Section 2.2.3.4).

b. Particle Swarm Optimisation

Particle Swarm Optimisation (PSO) is a class of swarm system that was initially inspired by flocks of birds and shoals of fish. The position of the particles represent solutions in the search space. The particles move through the search space tracking the current optimum particle. The method was conceptualised by Kennedy and Eberhart (1995) for the simulation of social behaviour. Only in a later publication was the algorithm recognised to serve as an optimisation algorithm (Kennedy, et al., 2001).

Throughout each iteration or timed step of the algorithm, the velocity of the particle is changed. This is achieved as follows:

1. Define an end condition (time or number of iterations).
2. Define maximum velocity, starting velocity and number of particles.

3. Randomly assign a starting position for each particle.
4. While end condition has not been met:
    a. Calculate the fitness value for each particle. If a value is better than the current best solution, save the new solution as the best solution.
    b. Calculate the velocity for each particle.
    c. Update the position of each particle using the new velocities.
5. Return the best solution.

Poli (2008) identified approximately 650 publications relating to the application of PSO within 26 fields including electronics, biomedical, design, finances, scheduling, forecasting and signal processing. The conclusion was that PSO performed well in most fields besides combinatorial optimisation problems due to premature convergence.

c. Artificial Bee Colony Optimisation

Like ACO and PSO, Artificial Bee Colony (ABC) optimisation is a swarm based algorithm which derives its fundamental concept from biology. ABC was conceptualised relatively recently by Karaboga, (2005). The algorithm mimics honey bees in search of food. Bees seek flower patches with high amounts of food that can be collected with minimal effort. Bees initially wander randomly between flower patches and when they return to the hive they evaluate their findings and communicate this information to the other bees. A bee will face the direction of the flower patch it previously visited and dance for a set time which indicates the distance and at a speed which indicates the quality of the patch. Bees from the hive interpret this information and follow the original bee back to the patch location if deemed suitable. The bees communicate their findings to the hive on every return so that locations with depleted food sources can be disregarded. This system ensures that patches with high amounts of food will be visited by more bees. Algorithmically this works as illustrated in Figure 2-8.

ABC has been successfully applied to a number of problems including software testing (Suri & Kalkal, 2011) and fault section estimation in power systems (Huang & Liu, 2013). Pham, et al. (2006) investigated 10 benchmark optimisation problems using ABC. They found that the method is comparable if not supperior to GA and

ACO in terms of speed and accuracy. For one particular test function, ABC converged to the same result 120 times faster than ACO and 207 times faster than GA. However, Huang and Liu (2013) stated "*reliability and flexibility of* [(ABC)] *has become the major concern which will be reported in the near future*".

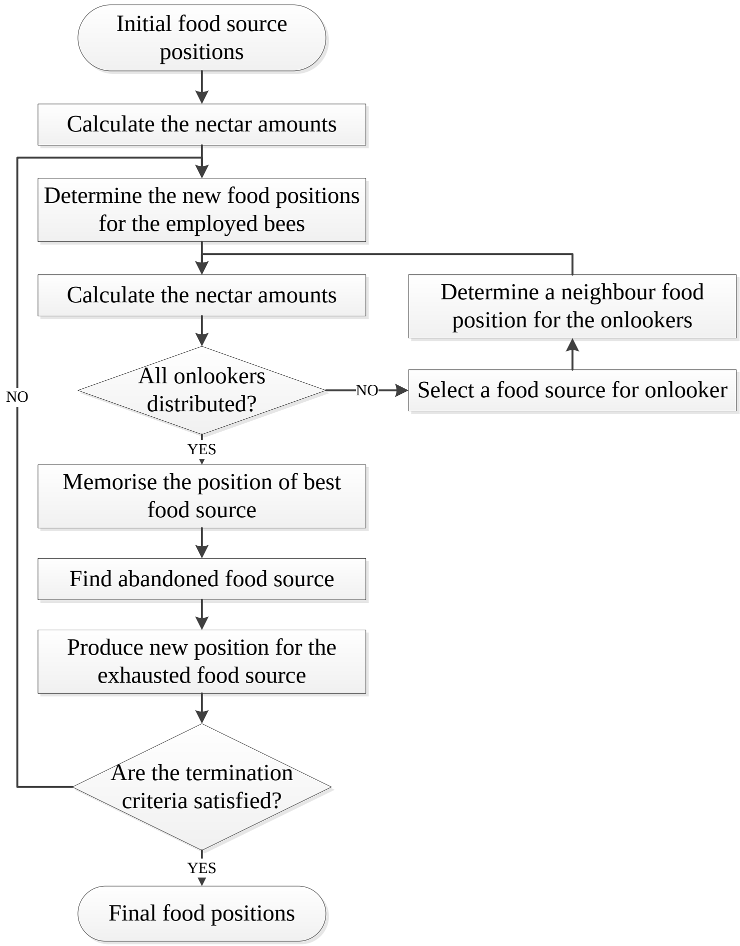


Figure 2-8 Flow chart of the ABC Algorithm (Karaboga, 2009)

2.2.3.4 Hybrid approaches

In recent years there has been much research conducted into combining MOO algorithms. Combining the advantages of two or more algorithms increases the chance of convergence to an optimum solution. Blum (2005) stated that hybrid algorithms typically provide better results than pure (singular) algorithms. Significant research has been undertaken with respect to combining algorithms that provide an extensive global search along with algorithms that perform an effective local search. From studying the work of Dawkins (1976), Moscato (1989) introduced the term memetic to describe a hybrid algorithm which utilises an additional technique for a local search.

As discussed in section 2.2.3.2, evolutionary algorithms are known to perform well for global searches but lack the ability of an extensive local search. With the combination of a gradient based local search technique, Moscato (1989) concluded a memetic approach has shown "*extraordinary performance dealing with some of the biggest instances of certain combinatorial optimization problems*". The memetic approach has also been applied to swarm based techniques. Petalas et al. (2007) successfully developed and reviewed a memetic based PSO algorithm. They found that "*in almost all problems the memetic approach proved to be superior, increasing both the efficiency and the effectiveness of the algorithm*".

Neri and Cotta (2012) conducted a review of memetic based applications. From the analysis, the authors stated that pure algorithms should not be separated into different fields but instead regarded as a "*combination of operators*". They proposed that the next step for memetic computing is to generate automatic combinations of optimisation algorithms.

2.2.3.5 Comparison and Summary

The MOO methods discussed have been used to address many different decision problems. There are a number of benchmark studies that evaluate the effectiveness of the various methods. However, these studies only demonstrate the algorithmic ability with a small number of specific problems. The best MOO results come from combining MOO methods. This has been confirmed for memetic type algorithms that use one MOO method for a global search and another for the local search.

2.2.4 Multi-Attribute Methods

Multi-attribute (MA) methods create a single numerical output to score each available alternative. This is achieved in two stages. Firstly, the decision-maker must identify and form sets of alternatives, criteria and decision variables which describe their decision problem. Secondly, a method which utilises a value or utility function is applied to aggregate this information into a final score. MA methods are generally categorised as either Multi-Attribute Value Theory (MAVT) or Multi-Attribute

Utility Theory (MAUT) approaches. Analytical Hierarchy Process (AHP) which works with pairwise comparisons is sometimes classified separately. However, Dyer et al. (1992) and a number of other publications classify AHP as a MAUT approach. Although a number of authors have laid claim to establishing the concepts of MAVT and MAUT, it is generally accepted that Keeney and Raïffa (1976) were the first to introduce the concepts. The main difference between MAVT and MAUT is that the former deals with problems under certainty while MAUT deals with problems under uncertainty. MAUT incorporates uncertainty through the use of utility functions as opposed to value functions. Both MAVT and MAUT only use criterion input on a common scale, consequently the functions which represent the decision problem must effectively normalise the decision variables (quantitative or qualitative) to a dimensionless common format. The way in which this is implemented for a particular method defines the method itself. The following section presents and explains the most commonly applied techniques that utilise MAVT or MAUT.

2.2.4.1 Weighted Sum

The Weighted Sum Method (WSM), also known as the Simple Additive Weight method, was introduced by Zadeh (1963). It is simple to understand and straightforward to apply, and has been evaluated in a range of fields hence it is one of the most widely applied MA methods (Chou, et al., 2008).

The WSM allows the decision-maker to define criteria weights. Each weight signifies the importance of a function. The total score of each alternative is equal to the sum of the product of the weights and decision variables:

$$A_i = \sum_{j=1}^{n} w_j a_{ij} \qquad for\ i = 1,2,\dots,m. \tag{2-7}$$

where a decision problem has m fixed alternatives and n fixed criteria. w_j denotes the weight of each criterion and a_{ij} is the decision variable for the i^{th} alternative with respect to the j^{th} criterion.

Even though the WSM has been widely used, the method itself is incapable of handling problems with multiple scales (Pohekar & Ramachandran, 2004). One solution is the application of normalisation procedures prior to applying the WSM.

However, there is no version of the WSM which incorporates a normalisation procedure into a single mathematical framework.

2.2.4.2 Pairwise Comparison Methods

The Analytic Hierarchy Process (AHP) (Saaty 1972; 1980) was proposed as a method to solve decision problems using a hierarchical structure of criteria and alternatives. AHP has become one of the most popular decision-making methods due to the use of pairwise comparisons to input qualitative information. Pairwise comparisons are required in the scale of 1-9. 1 infers equal importance, 3 for moderate importance, 5 for strong importance, 7 for very strong importance and 9 for extreme importance. The values of 2, 4, 6 and 8 are compromises between the previous definitions.

Pairwise comparisons given by the decision-maker are placed into reciprocal matrices. For example, a reciprocal matrix with 4 alternatives (a1,..,a4) is as follows:

	a1	**a2**	**a3**	**a4**	**Priorities**
a1	1	1/4	4	1/6	0.112
a2	4	1	4	1/4	0.248
a3	1/4	1/4	1	1/5	0.059
a4	6	4	5	1	0.581

Figure 2-9 Example reciprocal matrix in AHP

Values from the decision-maker for each pairwise selection are placed into the matrix and inverses are automatically added in the transpose position. The priorities are the principle eigenvectors of the matrix. Separate reciprocal matrices with alternative pairwise selections are required for each qualitative criterion. A score (in a numerical format) for each alternative is also required in respect to each quantitative criterion. The quantitative scores are normalised for the analysis. The priority values from the qualitative input and the normalised values from the quantitative input are used to form a score for each alternative by applying the WSM (equation 2-7). The criteria weights can either be collected as numerical values or from pairwise selections (in the same way as above).

Saaty (1980) acknowledged that intransitivity can occur when providing pairwise comparisons. For instance, a decision-maker can be intransient when expressing A is better than B, B is better than C and C is better than A. The decision-maker can also be numerically inconsistent by the decision-maker expressing A is better than B by 2, B is better than C by 2 and A is better than C by 6. Saaty (1980) consequently suggested the use of a Consistency Ratio (CR) to check that pairwise input is transitive. A CR works by quantifying how consistent the decision-maker's judgements are in relation to a large sample of random judgements (discussed further in section 4.5.2.2). Saaty (1980) proposed that if the CR is larger than 0.1 then the decision-maker's input is intransient and therefore unreliable.

AHP has also been scrutinised for an inherent limitation termed rank reversal. Rank reversal occurs when a new alternative is added or removed from the decision model after preferences have been provided. If the alternative preferences are close in the newly formed model, the update can alter the results, sometimes reversing the order of preference. This occurs due to interdependencies within the eigenvector calculations. Saaty (1980) suggested a technique termed supermatrix to overcome rank reversals in AHP. This technique, now commonly referred to as the Analytical Network Process (ANP) (Saaty, 1996), differs from AHP as it uses a network structure of criteria and alternatives rather than a hierarchical structure. The idea was that ANP would consider the interdependence of each criterion thus making the rank reversal problem void. However, Salo and Hämäläinen (1997) stated "*despite claims to the contrary, the supermatrix technuique* [(ANP)] *does not eliminate rank reversals*". The most sensible approach to ensure rank reversals do not occur is by ensuring the alternatives and criteria are correct before data entry (Saaty, 1994). This can be achieved by focussing on the problem structuring phase of the decision-making process.

There are a number of distinct differences between AHP and ANP which are shown in Table 2-1. As a consequence of the network structure of ANP, the decision-maker must input a much greater amount of information than when implementing AHP. This is potentially the reason why AHP has been applied and cited much more than ANP in recent years (Figure 2-4). The primary advantage of ANP over AHP is that "*dependence and feedback*" can be considered in the decision problem (Sipahi & Timor, 2010). Sipahi and Timor (2010), who discussed the recent developments of AHP and ANP, expect ANP to gain more popularity in the future. However, the AHP method is still the most cited method in the last decade out of all MCDA methods.

Table 2-2 Comparison between AHP and ANP

	AHP	ANP
Structure:	Hierarchy	Network
Pairwise Input required:	Medium	High
Considers dependence or feedback between elements:	No	Yes
Applications/citations:	High	Low/Medium

2.2.4.3 Ideal point methods

Ideal point methods assess alternatives on the basis of their separation from an ideal point. The two most prominent ideal point methods are Technique for Order Preference by Similarity to Ideal Solutions (TOPSIS) and VIKOR. TOPSIS was proposed by Hwang and Yoon (1981, 1995). The principle behind the method is that the optimal alternative should have the shortest distance from the positive ideal solution and the furthest distance from the negative ideal solution. The positive and negative ideal solutions are artificial alternatives which are hypothesised by the decision-maker, based on the ideal solution for all criteria and the worst solution which possesses the most inferior decision variables. For example, in terms of profit, a best solution could be £1 million and a worst solution could be £0. Assuming every criterion has an increasing or decreasing scale, TOPSIS calculates the results by comparing Euclidean distances between the actual alternatives and the hypothesised ones.

VIKOR, which was independently developed by Opricovic (1998), is a similar method to TOPSIS. The acronym in Serbian translates to "Multi-criteria Optimisation and Compromise Solution". Opricovic and Tzeng (2004) identified two differences between TOPSIS and VIKOR. They stated that "*a comparative analysis shows that these two methods use different normalizations and that they introduce different aggregating functions for ranking*". In terms of normalisation, TOPSIS uses vector normalisation whilst VIKOR uses linear normalisation to eliminate criteria measurement units. In terms of aggregation, TOPSIS attempts to evaluate the alternative with the maximum distance to the negative ideal solution while VIKOR tries to evaluate the alternative closest to the positive ideal solution (Chauhan & Vaish, 2012).

Similarly to AHP and ANP, both VIKOR and TOPSIS suffer from rank reversals. Nevertheless, both TOPSIS and VIKOR have been applied to a number of engineering problems such as materials selection (Chauhan & Vaish, 2012) and vehicle fuel selection (Tzeng, et al., 2005).

2.2.4.4 Comparison and Summary

Very few studies exist that compare Multi-Attribute (MA) methods. This is due to the differences between the inputs required from the decision-maker for each approach (i.e. decision variables, pairwise comparisons and ideal points). Much of the literature surrounding the comparison of MA methods is based on biased arguments with no substantive evidence. For example, one discussion between Smith and Winterfeldt (2004) and Gass (2005) compared AHP to alternative MAUT methods. Smith and Winterfeldt (2004) described AHP as "*fundamentally unsound*" due to the issues assosiated with measurement scale and rank reversals. Gass (2005) responded by contending that there are many successful applications of AHP and he urged the decision-making community to consider the method as one of the founding MA approaches. The only consensus is that most MA methods tend to reach the same decision outcome under the same conditions (Huang et al., 2011).

2.2.5 Outranking Methods

Outranking methods are commonly referred to as methods from the French or European school of thought. This is a consequence of the theory being introduced by the French Professor, Bernard Roy (1968). Accordingly, the literature regarding outranking methods is predominantly written in French. Recently due to the increased interest in decision-making, some of the original literature has been translated into English. This section introduces and reviews the most widely reported outranking approaches.

2.2.5.1 ELECTRE Family

ELECTRE stands for "ELimination Et Choix Traduisant la REalité" which in English means "Elimination and Choice Expressing Reality". Since the initial description of the technique in Roy (1968), seven further methods have been proposed, ELECTRE I, IS, Iv, II, III, IV and Tri.

ELECTRE I (Roy, 1968) is the simplest form of ELECTRE. The method uses concordance and discordance indices which are calculated for every possible pair of alternatives. A concordance index expresses how many criteria are in favour of each alternative and a discordance index expresses how many criteria are not in favour of each alternative. Using threshold values provided by the decision-maker, it is possible to determine if each alternative pair is preferred, indifferent or incomparable. By evaluating which alternatives are preferred more than not being preferred, the most promising alternatives can be identified. ELECTRE IS (Roy & Skalka, 1984) is exactly the same as ELECTRE I but it introduces an indifference threshold (the value below which the decision-maker is indifferent between two alternatives). ELECTRE Iv (Maystre, et al., 1994) is also similar to ELECTRE I but introduces a veto threshold (the value at which the decision-maker ultimately prefers one alternative over another and wishes to select that alternative with total certainty).

ELECTRE II was introduced by Roy and Bertier (1973) as the first modification of ELECTRE to deliver a full ranking of results. To achieve this, the concordance index was adapted to accept two levels of outranking relations, strong and weak, resulting in multiple threshold values being required. The complete rankings are calculated through two distillations procedures, one in descending order (finding the best to worst alternatives) and the other in ascending order (finding the worst to best alternatives). The final order is produced by taking an intersection of the descending and ascending orders (section 4.5.2.4).

Unlike the previous versions of ELECTRE, ELECTRE III (Roy, 1978) uses pseudo criteria to derive the concordance and discordance indices. Pseudo criteria are a fuzzy (Zadeh, 1965) representation of each criterion thus the method is capable of dealing with uncertain and limited information. Pseudo criteria are incorporated through the use of indifference, preference and veto thresholds. The indifference threshold is a value below which the decision-maker is indifferent in terms of two alternatives whilst the preference threshold is a value above which the decision-maker prefers one alternative to another. Finally, veto threshold is the value at which the decision-maker ultimately prefers one alternative over another and wishes to select that alternative with total certainty. The ranking of ELECTRE III is derived in the same way as ELECTRE II.

ELECTRE IV (Roy & Hugonnard, 1982) was proposed to simplify the procedure of ELECTRE III. In all of the aforementioned ELECTRE methods, the decision-maker assigns criteria weights. However, in ELECTRE IV, the threshold values are used to define a weighting scheme.

The final ELECTRE method, ELECTRE Tri (Yu, 1992) is an adaptation of ELECTRE III. It was proposed to categorise alternatives rather than provide a ranking. Categories (also commonly referred to as groups or classes) are established by the decision-maker and are ordered, typically in the arrangement of worst to best. The outranking relation is formed by comparing the alternatives to thresholds which are equivalent to the boundaries of each group. This provides the necessary information to categorise the alternatives.

The number of ELECTRE methods can be somewhat overwhelming. However, the methods can be categorised into three groups; choice (I, IS, Iv), ranking (II, III, IV) and sorting (Tri). In terms of modern decision support, the most useful group of methods is ranking. Within this group, Sayyadi & Makui (2012) recommend ELECTRE III as the most superior method as it can directly deal with uncertainty and gives the decision-maker the control to set criteria weights.

2.2.5.2 PROMETHEE Family

The Preference Ranking Organisation Method for Enrichment Evaluation (PROMETHEE) was introduced by Brans (1982). Like ELECTRE, the PROMETHEE family contains many versions which have evolved since the initial publication. The main difference between PROMETHEE and ELECTRE is that each independent criterion is associated with a preference function as opposed to a threshold value. Unlike a utility function in MA methods, the preference function is used to model the difference between each pair of alternatives. Six criterion types are defined as preference functions as shown in Figure 2-10, Usual Criterion (I), Quasi-Criterion (II), Criterion with Linear Preference (III), Level Criterion (IV), Criterion with Linear Preference (V) and Gaussian Criterion (VI). For each criterion function, one or two parameters need to be defined by the decision-maker, indifference threshold (q), preference threshold (p) and/or an intermediate value between q and p (s). PROMETHEE uses the preference functions to calculate positive and negative preference flows for each alternative, the positive flow expressing dominance and the negative flow expressing the weakness of each alternative against all other alternatives.

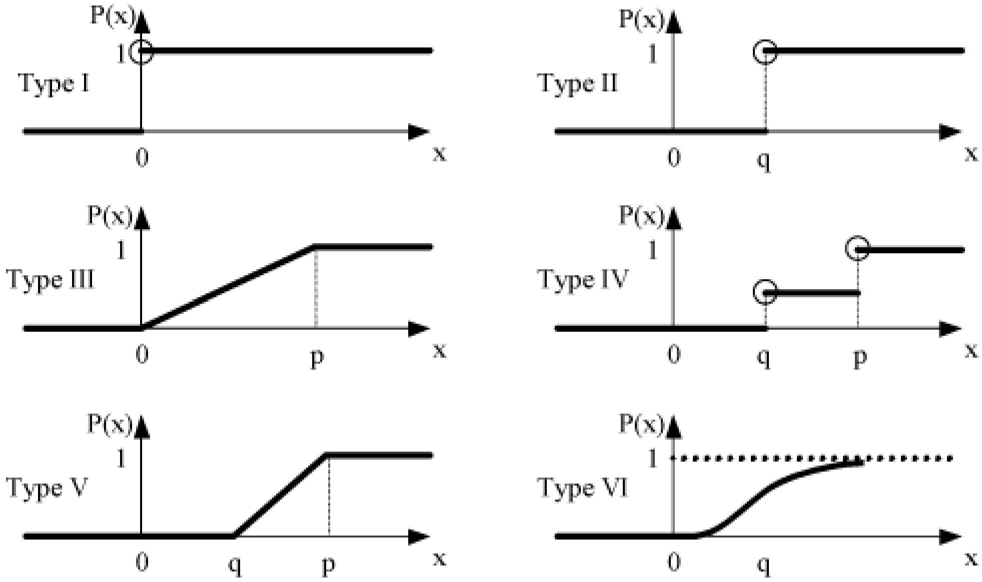


Figure 2-10 PROMETHEE Preference Functions (Dias, et al., 1998)

One advantage of the PROMETHEE method is that the output can be represented graphically by a technique called Graphical Analysis for Interactive Assistance (GAIA) (Mareschal & Brans, 1988). In GAIA, alternatives are represented by points while the criteria are denoted by the axes of the chart as shown in Figure 2-11.

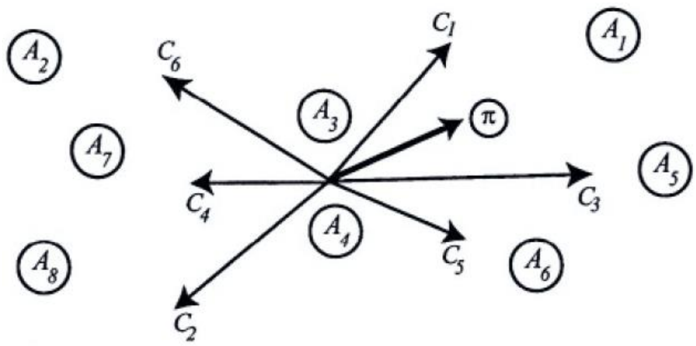


Figure 2-11 Example of GAIA Plane (Brans & Mareschal, 2005)

Criteria expressing similar preferences are represented by axes oriented in approximately the same direction (for example, in Figure 2-11, C4 and C6). Criteria expressing conflicting preferences are orientated in opposite directions (for example, in Figure 2-11, C1/C3 and C2/C4). Furthermore, alternatives that perform well with certain criteria are represented by points located in the direction of those criteria (for example, in Figure 2-11, A1, A5 and A6 perform well in terms of C1, C3 and C5).

PROMETHEE I and II were described in Brans (1982). Similar to ELECTRE I, PROMETHEE I can indicate the most promising alternatives while PROMETHEE II can provide a full ranking. The less cited methods of PROMETHEE III to VI, Tri and Cluster were proposed later. PROMETHEE III (Brans, et al., 1984) associates an interval with each action (rather than a preference flow) to highlight the notion of indifference. PROMETHEE IV (Brans, et al., 1984) provides a ranking when the set of viable solutions are continuous. PROMETHEE V (Mareschal & Brans, 1992) utilises constraints to maximise the total outranking flow of the alternatives in a continuous problem. PROMETHEE VI (Brans & Mareschal, 1995) allows for a range of variations in the criteria weights. PROMETHEE Tri (Figueira, et al., 2004), similarly to ELECTRE Tri, can be used to sort alternatives. PROMETHEE Cluster (Figueira, et al., 2004) can be used for nominal classification (sorting alternatives into groups).

Behzadian et al. (2010) reviewed over 200 publications relating to PROMETHEE. They noted that PROMETHEE has been applied to many business management, chemistry and manufacturing problems. However, no reference is made as to how PROMETHEE compares to other methodologies.

2.2.5.3 ORESTE

The "Organisation, Rangement Et Synthèse de données relaTionElles" (ORESTE) method was proposed by Rubens (1980) as an alternative to ELECTRE. The method works in the reverse manner to ELECTRE in that it forms a full order ranking of the alternatives then updates the order using threshold values. As a consequence, the ORESTE procedure requires only a weak order of alternatives and a ranking of the criteria in terms of importance from the decision-maker (Guitouni & Martel, 1998).

The procedure works by forming preference structures in an incomparability and indifference analysis. More specifically, when (A, B) is almost equal to (B, A) for every criterion then the comparison is incomparable (*R*). When (A, B) is much better than (B, A) for some criteria and (B, A) is much better than (A, B) for the remaining criteria, the comparison is indifferent (*I*). To make a distinction between indifference, incomparability and preference, three thresholds are computed β, δ and γ. The procedure for forming preference structures is summarised in the flowchart, Figure 2-12.

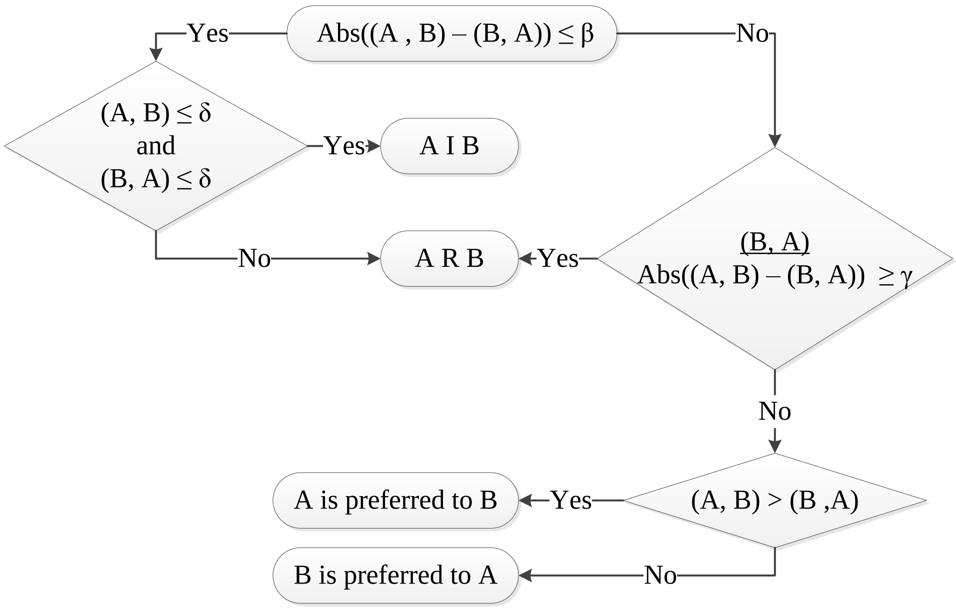


Figure 2-12 ORESTE Preference Structures (Bourguignon & Massart, 1994)

The main advantage of ORESTE over ELECTRE and PROMETHEE is that criteria weights are not required from the decision-maker as they are derived from the computed threshold values.

2.2.5.4 Outranking Comparison and Summary

Similar to MA methods, there are few comparative reviews or benchmark studies of outranking approaches. Only one review was located from an extensive literature search that recommended ELECTRE III over PROMETHEE II. Salminen et al. (1998) recommoned ELECTRE III since PROMETHEE II had "*no superior features when compared to it*". They stated that "*proportional thresholds for imprecise data of ELECTRE III were considered heavily in its favour*".

2.2.6 Other Techniques

The following section will discuss additional techniques that can potentially be used for decision-making. Firstly, two monetary based techniques are discussed, Cost-Benefit Analysis (CBA) and Cost-Effectiveness Analysis (CEA). Secondly, Bayesian methods are discussed with regard to three practical applications: decision trees, influence diagrams and belief nets. Lastly, game theory is introduced and discussed from a decision-making perspective.

2.2.6.1 Monetary Based Techniques

The following section introduces two techniques that can be used for economic evaluation; cost-benefit analysis and cost-effectiveness analysis.

a. Cost-Benefit Analysis

Cost-Benefit Analysis (CBA) evaluates the costs and benefits of alternatives using monetary values. Campbell and Brown (2003) described CBA as "*a process of identifying, measuring and comparing the social benefits and costs of an investment project or program*". The technique has been used extensively for guiding public projects (Brent, 2006), for example building motorways or discontinuing railway lines. The aim of CBA is to maximise the difference between benefits and costs which are transformed into a single dimension, net present value. For example, if a project has a benefit of 90 and a cost of 75, it should be approved, while if the cost was 100, the project should be rejected. The values for both cost and benefit are calculated from the value of money and time assosiated with each particular alternative.

CBA has also been used to evaluate environmental issues such as implementing policies to reduce pollution (Pearce, 1998). As a consequence, the United States Environmental Protection Agency released guidelines for economic analysis using CBA (US EPA, 2000). However, Pearce (1998) argues that CBA is not suitable for environmental decision-making. He stated that CBA "*can, at best, inform decision-making*". He also claims there are ethical implications as to whether all situations can be represented in monetary terms.

b. Cost-Effectiveness Analysis

Cost-Effectiveness Analysis (CEA) is a similar technique to CBA that does not simply assign a monetary value to an outcome. Instead a ratio is used of cost over effectiveness. Cost is represented again by net present value and the measurement for effectiveness is chosen by the decision-maker. The method is popular throughout the medical industry as patients' health benefits are difficult to express as monetary values (Donaldson, et al., 2002). The problem with CEA is that, similarly to costs, effectiveness must be utilised on a common scale. This greatly limits the use of the method as often effectiveness can be represented in a number of ways depending on the situation.

2.2.6.2 Bayesian Techniques

Bayesian techniques and the idea of conditional probability were conceptualised by Thomas Bayes (1763). If *A* and *B* are events, conditional probability relates to the parameter estimation of *A* given that event *B* occurs, written as $P(A|B)$. The Bayesian approach has become a common technique for reasoning under uncertainty. This section will focus on three practical Bayesian applications related to decision analysis: decision trees, influence diagrams and Bayesian belief networks.

a. Decision Trees

Decision trees were proposed initially in Von Neumann and Morgenstern (1947) for modelling games. The idea is that controllable events (decisions, depicted by rectangles) and uncontrollable events (probabilities, depicted by circles) are connected by branches in successive order to a set of outcomes (Figure 2-13). The trees can either be drawn vertically (top to bottom) or horizontally (left to right). The example in Figure 2-13 illustrates a horizontal decision tree showing the various market outcomes from two controllable investment decisions (the first for an initial investment and the second for a commercialisation investment) and two uncontrollable events.

Decision trees are particularly useful in working backwards to identify the expected value of certain scenarios. The only limitation of decision trees is that they can only be used with problems that are sequential in nature.

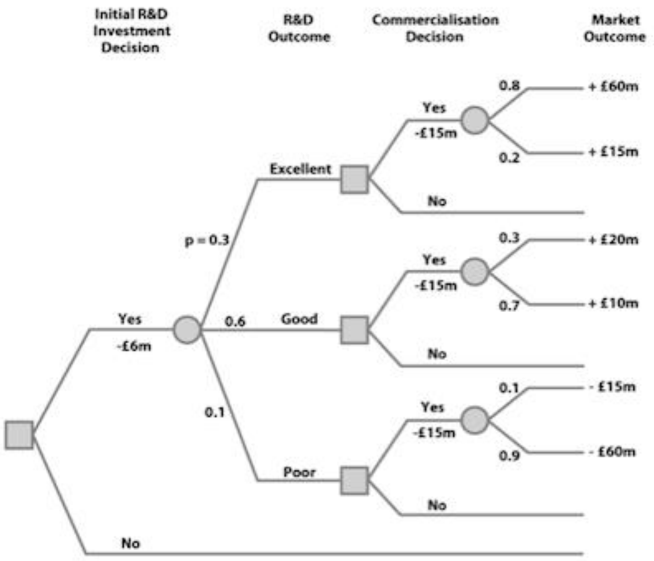


Figure 2-13 Investment Decision Tree Example (UCL, 2012)

b. Influence Diagrams

Influence diagrams expand on decision trees, with the aim being to formulate problems into a compact representation of information in a hierarchical structure. Similar to decision trees, there can be nodes that represent variable events in the form of controllable decisions (rectangle) or uncontrollable probabilities (circles). However, there also can be deterministic nodes (circle within another circle) and outcome nodes (octagons). Nodes are connected by a one directional arrow termed an arc which represents the "influence" between the two nodes. Figure 2-14 shows an influence diagram of an investment decision guided by a coin toss. As the decision does not directly influence the coin toss, there is no arc between the two nodes. However, since the uncertain coin toss is defined before the outcome, an arc from the coin toss connects to the payoff node.

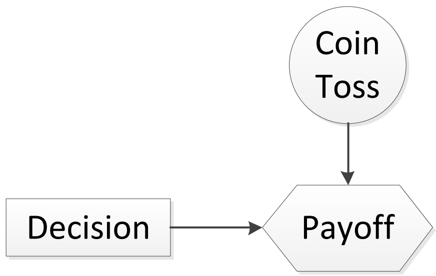


Figure 2-14 Example Influence Diagram (Marks, 2004)

c. Belief Networks

Belief networks are commonly known as expert systems that have emerged from the field of artificial intelligence. Although the technique shares similarities with decision trees, the method is more advanced and computationally intensive. Kjærulff and Madsen (2008) define a belief net as a "*Directed Acyclic Graph (DAG) which defines a factorisation of a joint probability distribution over the variables that are represented by the nodes of the DAG, where the factorisation is given by the directed links of the DAG*". In other words, a belief network contains a number of nodes which can vary in complexity from discrete variables to continuous multidimensional distributions. Nodes are connected (similarly to influence diagrams) by a one directional arrow called a link which implies a dependency relationship between two nodes. Figure 2-15 shows an example transport problem using a belief network with three uncertain criteria: journey time, waiting time and comfort. There are also five factors that influence the criteria, including: roadworks, train problems, start time, weather and transport type. The known factors can be used to calculate values for the uncertain criteria.

A belief network is useful to calculate evidence of belief for occurrences of unobserved events. However, large networks become difficult to manage as the information required to infer the conditional probability of certain nodes becomes extensive.

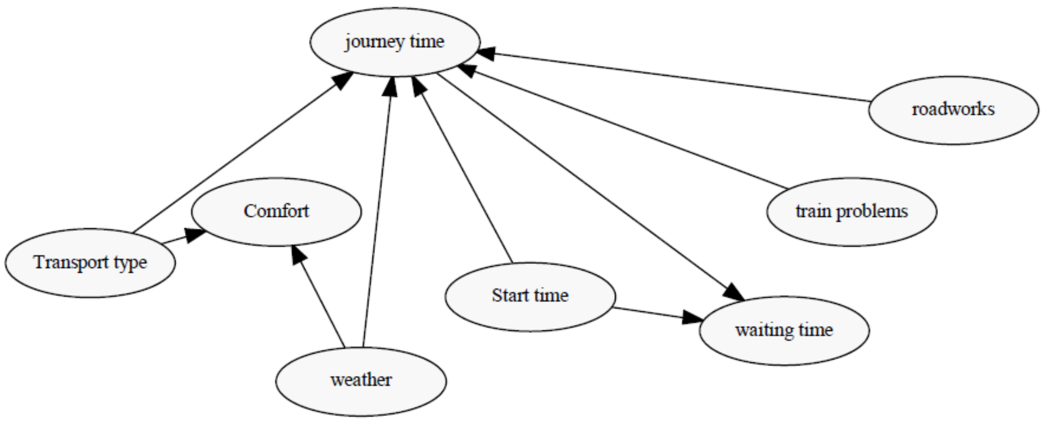


Figure 2-15 Bayesian Belief Network Example (Fenton & Neil, 1999)

2.2.6.3 Game Theory

The notion of game theory can be traced back to 1838 but only became popular within academia upon publication of Von Neumann and Morgenstern (1947) (Turocy

& Stengel, 2001). Much of the technical theory is closely linked to decision analysis, probability theory and Bayesian statistics. Game theory involves analysing strategies where one's success is somewhat affected by the choices of others (for example poker or chess). Clearly, the complexity of the problem increases in the case of cooperative or multi-player games.

Thomas J. Watson, the founder of IBM declared "*Business is a game - the greatest game in the world if you know how to play it*" (McMillan, 1996). Besides the ethical implications of this statement (considering games involve deceit, including bluffing or lying by omission), which are discussed by Koehn (1997), it is generally accepted that business decision-making is very similar to analysing alternatives in a game of strategy. Indeed, Von Neumann and Morgenstern (1947) stated "*the typical problems of economic behaviour* [are] *strictly identical with the mathematiacal notions of suitable games of strategy*".

Game theory research has not provided any tangible methodologies for application in decision support but rather a collection of beliefs or strategies that use the methods and techniques discussed in this chapter. The theories may potentially be useful in the identification of criterion, alternatives or decision variables from other peoples' (or rival companies) perspectives to earn a strategic advantage. Nevertheless, French (2007) suggests game theory and negotiation theory are full of contradictions and counterexamples.

2.3 Behavioural Decision-Making

The following section discusses developments in cognitive decision-making, examines decision-making in groups and reviews the mathematical theories that deal with irrational behaviour.

2.3.1 Intuition and Rational Thought

A book by Gladwell (2005) recommends the use of intuition to make decisions. It reports some interesting accounts of unconscious decision-making which been successful in a range of fields such as science, medicine, advertising and the music industry. However, most of the technical evidence is presented by Gigerenzer (2007). Both authors argue that acknowledging gut feeling (intuition) is a more effective way to make decisions than using sophisticated and complex computational models. The authors discuss the concept of unconscious intelligence which originates from ones previous experiences. This concept draws on the work of Simon (1992) who describes intuition as "*nothing more and nothing less than recognition*". Gigerenzer (2007) introduces the notion of 'rules of thumb'. A rule of thumb is described as a level of behaviour, reasoning or perception that is formed from conscious or unconscious understanding.

A number of scientific studies have endeavoured to evaluate the aforementioned theories on intuition. Dijksterhuis et al. (2006) found that in a problem relating to car selection, volunteers select better vehicles (based on a number of criteria) using intuition over conscious thought. However, two research groups challenged these findings by conducting similar experiments. Lassiter et al. (2009) repeated the same experiment but prohibited the volunteers from making an immediate decision. The results revealed the participants made better choices when provided with time for conscious thought. Cleeremans et al. (2009) also presented work of a similar nature utilising the decision of selecting an appropriate apartment. His work, similar to Lassiter et al. (2009) found that conscious thought was more likely to select alternatives with higher numbers of positive attributes.

Kahneman (2011) recently published his findings on thinking processes in decision-making. His work describes intuitive and conscious thought as two systems. System 1 is described as fast and effortless while system 2 is described as thinking slowly with high levels of contemplation. Kahneman (2011) acknowledges there are many problems associated with system 1 such as biases and overconfidence. He explains that people, especially experts, overestimate their understanding and underestimate the risk and uncertainty of complex decisions. Underestimating uncertainty is often fed by the certainty of hindsight rather than knowledge itself. Interestingly, he found the same people will also react differently to identical situations depending on what is on their mind. Nevertheless, Kahneman (2011) acknowledged system 1 for its ability to recognise patterns in a fraction of a second, for example reading an emotion from someone's facial expression or knowing the answer of 2+2 (but not 17 x 24). He explained that system 1 is particularly valuable when people achieve the ability to perform "*expert intuition*". This describes the phenomenon where experts have learned (from prolonged exposure to a particular situation) to train their subconscious pattern recognition mechanism to select the correct answer instantaneously, for example, doctors diagnosing a patient without any physical tests. Kahneman (2011) concluded by saying "*to block errors that originate in system 1 is simple in principle: recognize the signs that you are in a cognitive minefield, slow down, and ask for reinforcement from system 2*".

In conclusion, intuition should not be ignored; neither should it be followed without rational contemplation. For complex decisions which are significant to a person or a business it is imperative to consider, compare and contrast both intuition and structured conscious thought to deliver a coherent and rational solution.

2.3.2 Group Decision-Making

Often when companies are faced with complex decisions, the problem will be addressed by a group of people rather than one individual. Generally one would assume a simple voting system would be sufficient in handling such a task. However, literature from the fields of decision support, economics and psychology demonstrate many paradoxes and inconsistencies that criticise the idea of a democracy in decision-making (French, 2009). The most well-known criticism of democracy is Arrow's impossibility theorem (Arrow, 1963). Arrow's theorem shows that all current voting systems are either dominated by a single distinguished member or the member group as a whole delivers intransitive preferences (section 2.2.4.2). French (2007) states that no foundation for group decision-making exists that satisfies the principles of rationality, unanimity and Pareto optimality without there being an explicit or implicit dictator.

In terms of uncertainty, Kahneman stated that groups tend to be more overconfident and risk taking than individuals (Schrage, 2003). Stoner (1961) named this phenomenon "*risky shift*". Kahneman offers the explanation that individual doubts are frequently suppressed within a group and that groups which are susceptible to similar biases tend to be more optimistic which together leads to extreme outcomes.

Kahneman and French both suggest the practice of reflection within a group before implementing a decision outcome (Schrage, 2003, French, 2007). By doing this the decision attributes can be re-evaluated for inconsistences and some silent members of the group may voice their opposing opinion. French (2007) also suggests using an online individual voting system to collect information so single members are less likely to be influenced by a prominent or well-respected member.

2.3.3 Modelling Irrational Behaviour and Uncertainty

As discussed in section 2.2.1, expected utility theory has generally been accepted as the fundamental approach to handle choice under uncertainty. However, there has been considerable debate in the fields of economics and psychology which have uncovered a number of systematic violations of the expected utility hypothesis. For example, the Allais paradox (Allais, 1953) indicates that human reasoning can systematically violate expected utility theory. Considering the two decisions in Figure 2-16, Allais (1953) found that the majority of people chose option one over option two in decision one and option one over option two in decision two.
As the payoffs are dissimilar between these scenarios, Allais (1953) proves that people can be inconsistent (regardless of Utility, *U*):

$$\begin{aligned} &U(£1M) > 0.1*U(£5M) + 0.89*U(£1M) + 0.01*U(£0) \\ &0.1*U(£5M) + 0.9*U(£0) > 0.11*U(£1M) + 0.89*U(£0) \end{aligned} \qquad \textbf{2-8}$$

Decision 1	Option One:	Receive	£1M with a probability of 1
	Option Two:	Receive	£5M with a probability of 0.1
			£1M with a probability of 0.89
			£0 with a probability of 0.01
Decision 2	Option One:	Receive	£5M with a probability of 0.1
			£0 with a probability 0.9
	Option Two:	Receive	£1M with a probability of 0.11
			£0 with a probability of 0.89

Figure 2-16 Allais Paradox with a modified currency

Kahneman and Tversky (1979) repeated the Allais experiment with modified values to provide moderate rather than extremely large gains. They too concluded that human decision-making did not conform to expected utility theory. Kahneman and Tversky (1979) believed that "*decision making under risk can be viewed as a choice between prospects or gambles*" and thus introduced prospect theory (a method of non-expected utility). Prospect theory assigns values to gains and losses rather than to final assets. A reference point is used to define the value function to which gains are concave to imply risk aversion and losses are convex to imply risk taking (Figure 2-17).

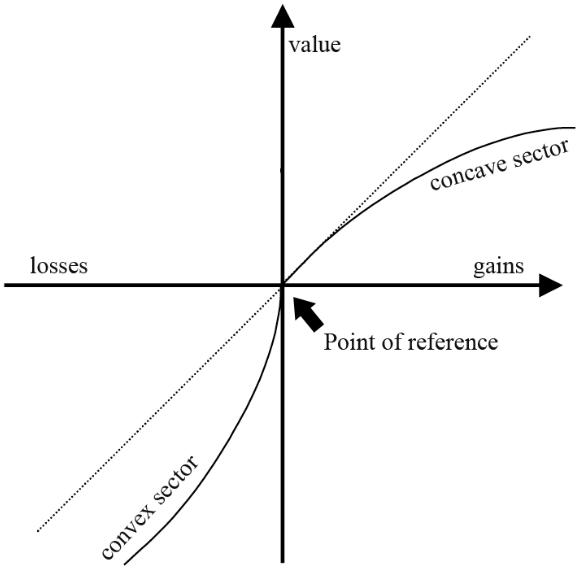


Figure 2-17 Illustration of a value function in Prospect Theory

Machina (2008) reviewed a number of preference functions (such as prospect theory) that have been used to model non-expected utility. Each approach differs and describes a function which is purported to infer human selection. As it is not known how the human brain functions under uncertainty (Trepel, et al., 2005) it is difficult to identify if there is a function which would accurately mimic human choice. Furthermore, Binmore (2011) believes that the methods of non-expected utility are not suitable for predicting the outcome of peoples' behaviour. He argues the theories have been calibrated based on hindsight (using experiments) thus they do not represent every situation. Additionally, he refers to two papers by Harless and Camerer (1994) and Hey and Orme (1994) which found that many of the non-expected utility theories provide inferior predictions of behaviour compared to expected utility theory itself.

It is clear from the aforementioned discussion that cognitive selection is not linear and a number of alternative methods, such as prospect theory, have been proposed which attempt to model human choice under uncertainty. However, these methods have been proven to be ineffective for certain problems and within certain contexts.

One alternative technique for compensating for uncertain selections is the use of fuzzy set theory which was proposed by Zadeh (1965). Classically, logic has been defined by two values, 1 or 0 and is termed crisp logic with an object being an element of a set or not. Fuzzy logic alternatively introduces the concept of membership. A fuzzy set in relation to a crisp set for the definition of "hot" is illustrated in Figure 2-18. As shown, in crisp logic, hot is defined between 20C and 50C while the fuzzy set expresses a membership of hot between 10C and 60C with only 35C being at a membership of 1.

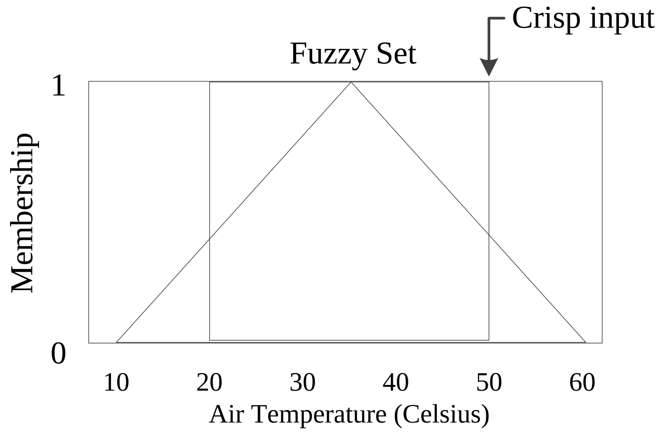


Figure 2-18 Example of a Fuzzy Set for the definition of "hot"

Fuzzy logic has been applied to a number of MOO, MA and outranking techniques to capture uncertainty. However, Stewart (2005) considers the fuzzy approach impractical for modelling human judgements. He states that "*such models of imprecision add complexity to an already complex process, and the result may often be a loss of transparency to the decision maker, contrary to the ethos of Multi-Criteria Decision Analysis*". Stewart (2005) suggests handling uncertainty by improved formulation of the decision problem and by conducting an appropriate sensitivity analysis. The most common form of sensitivity analysis in MCDA is to apply a local 'one-at-a-time' modification (Van Der Pas, et al., 2010). This involves changing one decision variable at a time to see how the output is affected and then returning the parameter to the decision-maker's baseline value.

2.4 Chemical Decision Literature

Following an extensive literature search, there are very limited references to decision-making techniques utilised for Whole Process Design (WPD). This is potentially due to the concept being relatively new and has been the domain of

Britest members. Therefore this section will focus on literature which aims to address management decisions associated with product or process development. The section is split into two parts, the first assesses Multi-Objective Optimisation (MOO) based applications whilst the other evaluates Multi-Attribute (MA) and outranking applications.

2.4.1 Multi-Objective Optimisation Applications

Literature on chemical management decision-making is dominated by the use of MOO methods (Grossmann, 2005). This is potentially a consequence of optimisation techniques being familiar as they have been widely applied in process control. MOO methods have been applied extensively to areas including supply chain management (Shah, 2005) and abnormal event management (Venkatasubramanian, et al., 2003). However, fewer applications exist that address decisions throughout product and process development.

The majority of the MOO based literature that covers decision-making within product and process development involves the inclusion of environment, health and safety (EHS) considerations. In the past, non-monetary issues of process design such as safety, worker's health and environmental impact were either not a systematic part of the decision-making process or were only considered at the final development stage (Adu, et al., 2008). However, with the growing awareness of legislation associated with EHS, a number of methodologies have been applied, including hazard and operability analysis (HAZOP) (Kletz, 2006), fault tree analysis (FTA) (Watson, 1961), failure mode effect analysis (FMEA) (Anon., 1980) and life cycle assessment (LCA) (Klopffer, 1997). These methods, although valuable require significant amounts of data and an advanced level of process understanding. At the beginning of product and process development when little data is available these methods are not viable (Adu, et al., 2008). Consequently, researchers have developed methodologies to incorporate EHS factors in the early development decision-making process.

Three independent research groups have developed methodologies linking EHS with product development decision-making utilising MOO methods. BASF (Saling, et al., 2002) proposed an Eco-efficiency Analysis for comparing product or process alternatives in terms of environmental impacts and costs. The analysis was based on an extended LCA according to ISO14040ff (Environmental Management: LCA:

Principles and Framework). Data related to the economic and ecological aspects of a system featuring different alternatives was normalised and aggregated to produce an Environmental Fingerprint (Figure 2-19) and Eco-Efficiency Portfolio (Figure 2-20).

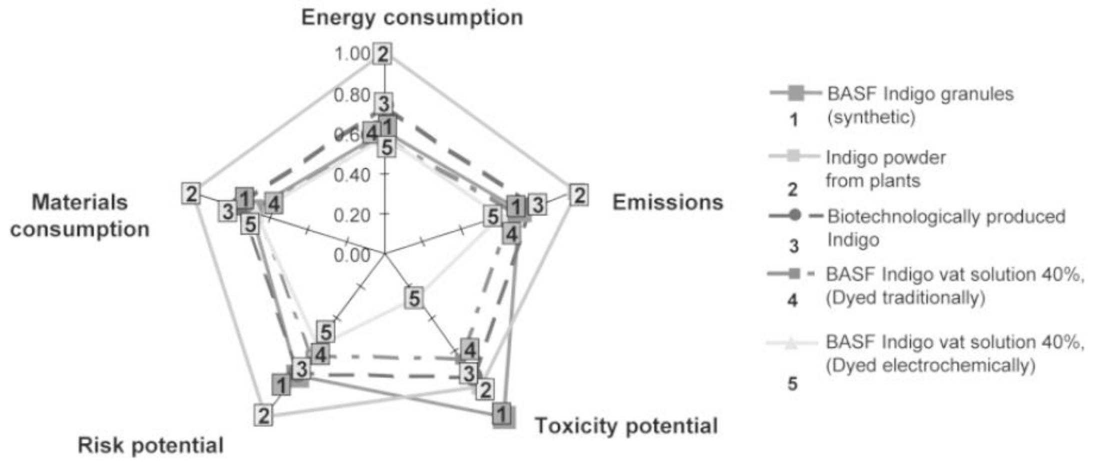


Figure 2-19 BASF Environmental Fingerprint Example (Saling, et al., 2002)

Figure 2-19 shows that the electrochemical option (5) is the most advantageous alternative in all categories except materials consumption and indigo powder from plants (2) is the least favourable alternative in all categories except toxicity potential. This can be seen in Figure 2-20 where the most favourable alternatives are located at the top right and the least favourable are located at the bottom left of the portfolio. The diagonal distance between the alternatives indicates the respective eco-efficiency.

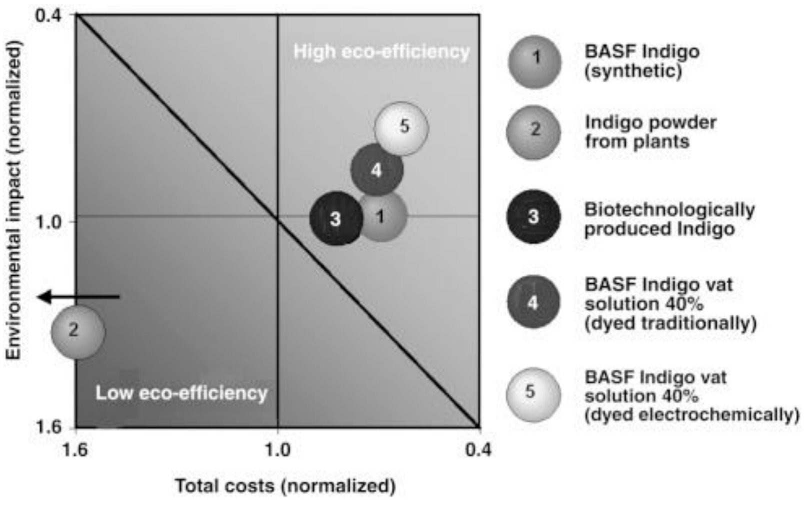


Figure 2-20 BASF Eco-Efficiency plot (Saling, et al., 2002)

The second framework proposed by Chen and Shonnard (2004) combines and optimises an economic index (net present value) with an environmental index (process composite environmental index) to give an environmentally concious design. The system works by combining an environmental fate and risk assessment tool with AHP. The output from this is optimised using a GA to identify the "best" design.

The final framework presented an early stage chemical process design assessment in relation to continuous processes (Sugiyama, et al., 2008) and later for batch processes (Albrecht, et al., 2010). Both systems work similarly by determining indicator values for the economic behaviour, environmental impacts and hazard potential for each alternative. The indicator values are aggregated into a single index value which is used to rank the alternatives.

Although these three works contributed significantly to the development of this field, shortcomings remain:

- Little or no reference is made with regard to the choice of a suitable MOO method. Chen and Shonnard (2004) proposed the use of GA because "*it provides a flexible, relatively efficient, and effective method for handling the black box*". However, they fail to evaluate or consider other MOO techniques. The other two frameworks do not cite any particular MOO algorithm.
- The frameworks proposed are well defined but require significant amounts of data and information that would be very timely to source and evaluate.
- The majority of the criteria are defined in terms of costs. However for some criteria such as those relating to safety and the environment, it is difficult to quantify them in terms of a monetary value.
- All three frameworks are difficult to modify. Every product and process development is different, hence flexibility is essential in terms of a framework that addresses these overarching challenges.

2.4.2 Multi-Attribute and Outranking Applications

The majority of the literature surrounding MA and outranking methods in chemical related journals are methodological reviews. Keller and Massart (1991) reviewed the Weighted Sum Method (WSM), Pareto Optimality, ELECTRE and PROMETHEE methods. The evaluation centred on a case study concerning the selection of a formulation for a textile product. The review described PROMETHEE as a "*more recent and more sophisticated solution*" than other methods. However, the results from the benchmark study indicated that all of the methods attained a similar outcome. Throughout the publication, the PROMETHEE method was endorsed without much support from the literature or the authors own results. The bias most likely was attributed to the third author being the creator of the PROMETHEE methodology.

Pirdashti et al. (2009) provided a further more substantial review of MA and outranking methods. They discussed techniques from both the European and American schools of thought but chose to only evaluate five of these methods; AHP, MAUT, ELECTRE, PROMETHEE and TOPSIS. In line with the findings reported in Figure 2-4, they acknowledged that AHP is the most popular decision-making method. The review provided no justification for selecting a particular method. Instead, the authors state that relatively little research has been published on the decision-making techniques that are actually used in companies and propose that the methods need to be tested in industry.

Pavan and Todeschini (2009) provided a further review of decision-making methods. Although the study covered many techniques including MAUT and outranking methods, the authors did not discuss AHP or ANP. Nor did they provide any justification for selecting a particular method.

Although the three reviews proposed a range of decision-making methods, only three approaches have been repeatedly applied to problems in the chemical decision-making literature, AHP, ANP and WSM. Terashi and Umeda (1991) presented a methodology for value system design where AHP was used to analyse design alternatives. Xiaoping et al. (2006) used AHP to evaluate alternatives in the context of sustaining a chemical industrial park. Partovi (2007) proposed a method combining AHP, ANP and Quality Function Deployment (QFD) for selection between batch and continuous chemical processes. Likewise, Ridder et al. (2008) proposed a method utilising ANP and QFD for Research and Development (R&D) decisions, in particular equipment selection. Leng et al. (2012) discussed the use of WSM for selecting a synthetic route for a new organic molecule. Similarly, George et al. (2007) applied a modified version of the WSM to a hypothetical example that considered acquiring a commercial scale biomanufacturing facility. The adjustment applied Monte Carlo simulations (Metropolis, 1987) to account for the uncertainty in the decision-maker's decision variables. The rationale was that the random nature of Monte Carlo enabled the evaluation of many scenarios thereby providing an an overview of the uncertainty in each option.

All the authors who used AHP and ANP concluded that the techniques are useful and straightforward to apply to many types of decisions but some of the authors stated that by using AHP, the analysis was time consuming due to having to evaluate a large number of pairwise comparisons. The authors who applied the WSM also found the technique useful due to the straightforward nature of the calculations. In all cases, none of the authors provided any justification for selecting a particular method.

2.5 Conclusions

It is clear from the literature that there are a range of methods available for decision support. However, there is no clear indication which methods would be the most effective for solving decision problems in the context of WPD. The overall aim of this chapter was to answer the following questions:

RQ2: Which methods in the literature are the most commonly cited/applied for solving multi-criteria decision problems? Furthermore, which of these methods are most suitable for handling uncertainty?

RQ3: Which methods in the literature have been proposed or used for decision-making in process design?

Therefore the conclusions are presented in two sections, addressing each question in sequence.

2.5.1 Methods and Uncertainty

The most commonly reported methods in the literature for multi-criteria decision support can be classified into three groups; MOO methods, MA methods and outranking methods. Each group has its own advantages and limitations. This section presents a benchmark study of these groups (Table 2-3). The benchmark was created using the literature discussed and the comparative studies of Malczewski (1999) and Linkov et al. (2006).

Table 2-3 Benchmark study of Decision-Making Methods Groups

	MOO Methods	MA Methods	Outranking Methods
Criteria defined by:	Objectives	Attributes	Attributes
No. of Alternatives:	Infinite	Finite (1-15)	Finite (1-15)
Decision Variables:	Quantitative only	Quantitative & Qualitative	Quantitative & Qualitative
Results:	Cardinal Value	Cardinal Value	Ordinal Rank
Results accuracy:	High	Moderate	Moderate
Method Complexity:	High	Moderate	High
Modelling time:	High	Low	Low
Ease of modelling Uncertainty:	Moderate	High	High
Ease of group decision-making:	Low	Moderate	Moderate
Relevant to	Search / Design	Evaluation / Choice	Evaluation / Choice

The benchmark study shows that MOO methods differ from MA and Outranking methods in multiple ways. MOO methods utilise objective functions in search or design problems to explore a vast number of solutions. As a consequence, modelling is complex and demands time from the decision-maker. Furthermore, MOO methods are unable to handle qualitative information, this makes the modelling of uncertainty difficult, particularly when decision-makers have limited knowledge or understanding of a selection. Alternatively, MA and outranking methods utilise qualitative and quantitative attributes to evaluate decisions and recommend choices. Subsequently, they are more suited to handling uncertainty than MOO methods but their results accuracy is lower. The only difference between MA and outranking techniques in the benchmark study is that MA methods output numerical results while outranking methods output an ordinal rank.

It is evident that there is no best MOO method despite the fact that an array different techniques have been proposed including goal programming, simulated annealing, evolutionary algorithms and swarm techniques. As of a result, memetic approaches which combine different algorithms for global and local searches have become popular. Similarly to MOO, the literature suggests there is no best MA method even though AHP has clearly received the most academic and industrial interest. However other methods such as WSM have become popular due its straightforward implementation. MA methods cannot be easily combined unlike MOO methods as the inputs required for each method differ. For example AHP requires pairwise comparisons while WSM requires direct decision variables. Therefore evaluating a single decision utilising different MA methods requires extended time and effort by the decision-maker. Outranking methods are limited to three method families with ORESTE receiving little interest in the literature. Of the two most commonly cited outranking methods, ELECTRE and PROMETHEE, Salminen et al. (1998) stated that ELECTRE III is more superior to PROMETHEE II due to its ability to model inprecise data using threshold values.

2.5.2 Methods used in Process Design

A number of decision-making methods have been proposed for application during product and process design. Three research groups have developed frameworks utilising MOO algorithms for optimising process design with environment, health and safety considerations incorporated. These frameworks have been proven to be useful for the specific case studies reported. However, the frameworks are complex and inflexible which may deter industry users from adopting them.

A number of researchers have reviewed and proposed the use of MA and outranking methods for management decision-making in the chemical-using industries. However, only three methods have been applied to real problems in the literature; Analytic Hierarchy Process (AHP), Analytic Network Process (ANP) and Weighted Sum Method (WSM). Potentially this is due to the fact that they are easy to implement and/or software is readily available (Huang et al., 2011).

The following chapter identifies the industrial requirements for developing a decision-making framework for use during Whole Process Design (WPD). In the subsequent chapters, these requirements will be compared to the methods presented in this chapter to identify an effective solution for decision-making in WPD.

"Biology is now widely considered to be a foundation science of chemical engineering. Will management be next?" **Ka M. Ng** (2004)

3 Industrial Requirement

3.1 Introduction

The previous chapter critically reviewed the academic literature to identify and discuss a range of methods available for decision support. This chapter aims to identify the industrial requirements for developing a decision-making solution for use in Whole Process Design (WPD) by considering the following three research questions:

RQ4: What techniques are currently being used for decision-making in industry?

RQ5: What are the most common decisions made in WPD and in what stage of development are they considered?

RQ6: What does industry require from a decision-making framework?

The approach adopted was to undertake a mixed methods practice. This involved carrying out two qualitative semi-structured interviews with senior industrial decision-makers. The goals of these interviews were to identify:

- the company's decision-making processes.
- the company's requirements for a decision-making framework.

The outcomes of the interviews identified further questions which were addressed through the circulation of two questionnaires to professionals within the chemical-using industries via Britest Ltd. The initial questionnaire focused on identifying the decision-making procedures used by professionals and determining the common problems faced in WPD. The goal of the second questionnaire was to identify the requirements for a decision-making framework. Together the data from the two methods generate complementary insights in accordance with the research questions.

3.2 Interviews

The two initial interviews were conducted with representatives from Robinson Brothers Ltd and British Petroleum plc (BP). Both interviews were semi-structured, allowing for flexibility with the questions and overall discussion. This encouraged two way communication, ensuring the topics discussed were understood by both parties. The interview with Robinson Brothers was completed face-to-face, while the interview with BP was achieved via teleconference.

Robinson Brothers is one of the UK's largest independent manufacturers of speciality organic chemicals and BP is a leading international oil and gas company. Robinson Brothers is a member of Britest Ltd and consequently has adopted a Whole Process Design (WPD) philosophy. BP is not a member of Britest and consequently have their own strategies in place for product and process development. The benefit of assessing the industrial requirements of Robinson Brothers and BP is that both companies are not members of Britest. Therefore, two contrasting perspectives were attained and thus ensured the outcomes in terms of identifying requirements for a decision-making framework were more general than if only Britest members were considered.

3.2.1 Robinson Brothers Limited

The interviewee at Robinson Brothers was a business and technical development manager whose background was originally in chemistry but had gained significant experience in chemical engineering. His focus at the time of the interview (12^{th} November 2009), was on acquiring business and increasing sales.

3.2.1.1 Decision-Making Process

The following information was articulated by the interviewee during a discussion on decision-making. Companies often approach Robinson Brothers to initiate a contract for the manufacture of chemical products. The interviewee draws on all the information available to him (chemical, engineering, business and previous experience) to reach a rational conclusion on whether to accept a contract and if so, to quote a price. Time is considered as an important aspect in the decision-making process as companies that require Robinson Brothers' products and services expect efficient and rapid turnaround of contractual decisions.

The first stage of the decision-making process is to perform a series of checks on a new proposal to identify potential issues. The basis of the checklist is a document that covers health and safety, known literature and government regulations. Any one of these could be a show stopper and result in the contract being turned down. The

next stage is to determine if there are any other reasons why the product should not be produced by Robinson Brothers. The interviewee uses “MSLE” (Materials, Service, Labour and Effluent) to prompt his thought process. Finally, other factors are considered such as the market, potential competition and who the customer is.
On deciding to make a bid for a contract, the interviewee considered the previous criteria and further quantitative criteria (such as material costs, labour costs and manufacturing time) to determine a price. This is challenging as under-pricing results in loss of profit and overpricing will result in the customers accepting a competitor’s offer, meaning Robinson Brothers will lose business.

3.2.1.2 Requirements for a Decision-Making Framework

Whether deciding to make an offer for a proposed contract or when deciding on a production price, many different criteria need to be considered including production time, government regulations, material costs, safety implications, product yield, market size, resource management, process knowledge and the customer’s geographic location. The challenge is that many of the criteria are in conflict. For example, safety implications could affect the lead time which in turn affects the price offered to the customer. The interviewee explained that he finds decision-making challenging and a tool that would allow him to organise his thoughts and ensure that all the various criteria are considered when reaching the final decision would be valuable. He also said that generating an exact recommendation is not important, however a decision-making tool that formulates his criteria and visualises the differences between his alternatives would be of benefit. He used the analogy that business is not “*black and white*” but ensuring his decisions are well thought through and based on all the information available would make his business decision-making “*less grey*”.

3.2.2 BP

The interviewee at BP was the Technology Vice President who has a professional Masters degree from Harvard Business School. His background at the time of interview (1st December 2009) was in chemical engineering, management and business. He was responsible for the development of a portfolio of technologies to create synthesis gas from a range of primary fuels. His role included applied research, pilot plant design/operation, technology licencing and project development leading to commercialisation.

3.2.2.1 Decision-Making Process

BP operates their product and process development decision-making processes under the Stage Gate^{TM} framework (discussed in section 1.1). There are four major milestones in BP's adaptation of the Stage Gate^{TM} process; appraise, select, develop and financial memorandum. At each gate, the decision-maker(s) can choose to stop, continue or recycle a project. Stopping a project means that it will be terminated completely, while recycling a project means it may be considered again at a later date.

At the first gate (appraise) the stop, continue or recycle decision is made considering only six criteria: time, cost, value, capability, risk and opportunities. At the second gate (select), the stop, continue or recycle decision is considered in greater detail by introducing further criteria related to financial, social and environmental aspects. To make this decision, a detailed report is created outlining the risks and includes a cost benefit analysis (discussed in section 2.2.6.1). At the third gate (develop), marketing plans are introduced, surveys are conducted and people are selected to manage the project. The final gate (financial memorandum) is where a project requires its final approval. As projects can cost anywhere from £10 million to billions, the decision made at the fourth gate is crucial.

3.2.2.2 Requirements for a Decision-Making Framework

The interviewee explained that the Stage Gate^{TM} framework works well for BP but he admits that due to the flexibility the system does have a tendency to increase development times contrary to what Cooper (2001) claimed (section 1.1). He explained that BP does not have any tools in place for analysing decisions however some employees use their own report checklists and/or spreadsheets to assist them.

When asked what requirements he would have for a decision support system, he requested the functionality to utilise past decision knowledge in future decisions.

3.2.3 Interview Outcomes

The interviews revealed that both companies deal with complex decision problems by taking into consideration multiple criteria and their interactions. The decision problems described are complex as they adapt to the interactions of various business and technical events, data and the collective subjective behaviour of the decision-maker(s) (Johnson, 2011). Both companies considered memory/feedback from previous decisions/events and consider the uncertainties from lack of knowledge and unknown present/future decisions/events. The companies have similarly developed procedures to review their decision problems. However, neither of the companies have any tools in place to help with addressing these complex decisions. On questioning, both companies revealed their requirements for a decision-making framework. These requirements can be summarised by the following five points:

- Both companies require a framework that will assist the decision-maker(s) in identifying the criteria that are relevant to their problem.
- Both companies require a framework that can be implemented rapidly. Robinson Brothers stated that turnaround in terms of whether to bid for a contract is crucial to their organisation while BP perceived that their Stage Gate^{TM} system resulted in increased development times.
- Both companies require a framework that can handle decision problems with a small number of alternatives. Robinson Brother's primary decision is to determine when to bid for a contract or not (2 alternatives) while BP's gate decisions are to select either stop, continue or recycle (3 alternatives).
- Both of the companies require a framework that can retrieve and reuse past decision knowledge.
- Robinson Brothers requested a framework that can formulate their criteria and visualise their alternatives rather than one that provides exact recommendations.

The above requirements indicate the relevance of a MA or outranking based decision-making framework as qualitative criteria are considered and the problems described consider only a few alternatives (section 2.2.3). However, identifying the requirements of only two companies is not sufficient to reach a consensus that is reflective of the entire process industry, especially in light of the fact that BP has not formally adopted the WPD philosophy. Therefore, further investigation is required to consider the applicability of the requirements identified above in the context of WPD.

3.3 Questionnaires

To increase the validity of the aforementioned research, two questionnaires were formulated to extend on the findings of the interviews. The results presented in this section were acquired from compiling the outcomes of two questionnaires that are presented in Appendix A. The first questionnaire (25^{th} January 2010 – 19^{th} February 2010) focused on identifying the decision-making procedures used by professionals and determining the common problems faced in WPD. The second questionnaire (8^{th} August 2010 – 27^{th} August 2010) concentrated on identifying the requirements for a decision-making framework. The questions in the first questionnaire were similar to those in the interviews while the questions in the second questionnaire were highly influenced from the interview and initial questionnaire's responses. Both questionnaires were conducted online and the responses were received in various formats. In the first questionnaire, questions required either/or answers, selection of an answers from a list and selection of importance using a 1-10 scale. A small number of open ended questions were used to gain a deeper understanding of the respondents' opinions. The second questionnaire was more straightforward with the majority responses requiring either/or answers with a few open ended questions. The broad range of formats used to collect answers in the two questionnaires gathered mainly definitive responses making the results quantifiable with only a small number of sensitizing responses leading to a deeper understanding.

The questionnaires were circulated to industrial decision-makers within Britest's membership who were employed at managerial level and made decisions pertaining to WPD. All of the respondents held postgraduate qualifications in either chemistry or chemical engineering. The preliminary ethical assessment form provided by Newcastle University specified that an ethical approval of the questionnaires was not required.

Twelve companies including Infineum, Fujifilm, Johnson Matthey, Robinson Brothers, Abbot, AMRI Global, Pfizer and Uetikon GmbH contributed to the studies. The remaining four companies requested to remain anonymous. In total, nineteen responses were received for the first questionnaire and fifteen responses for the second questionnaire with nine respondents providing answers to both (Table 3-1). The primary Standard Industrial Classification (SIC) code for each company has been included in Table 3-1 to give an appreciation of the domain area. Noticeably, there was an even distribution of businesses across the chemical and pharmaceutical sectors. Only two companies shared the same SIC code, Infinium and Robinson Brothers Ltd, who are manufacturers of other organic based chemicals.

Table 3-1 Companies who responded to each questionnaire

Company	Primary SIC Code	Questionnaire1	Questionnaire2
Infineum	Manufacture of other organic based chemicals (2414)	2	2
Fujifilm Colorants Ltd	Manufacture of other chemical products (2466)	4	1
Johnson Matthey Plc	Other business activities (7487)	3	2
Robinson Brothers Ltd	Manufacture of other organic based chemicals (2414)	3	1
Abbott Laboratories Ltd	Wholesale of pharmaceutical goods (5146)	1	2
AMRI Global	Commercial physical and biological research (8731)	0	1
Pfizer Ltd	Pharmaceutical preparations (2834)	0	2
Uetikon GmbH	Engineering activities and related technical consultancy (7420)	0	1
Anonymous	N/A	6	3

The results of the questionnaires have been separated into three sections, one for each of the research questions addressed in this chapter.

3.3.1 Techniques currently used for decision-making in industry

The respondents were asked to identify and explain the methods they currently utilise in decision-making. More specifically, two questions were asked, one relating to methods completed by hand and the other concerning the use of computational approaches.

3.3.1.1 Handwritten Decision-Making Methods

Seventy eight percent (78%) of the respondents reported that they use handwritten decision-making methods. A total of eleven approaches were cited (Table 3-2). A feature common to all the methods is that they can be used to graphically or pictorially brainstorm a decision problem. A number of them can also be used to identify suitable criteria and alternatives. A limitation of the methods is that none of them provide a means to provide a solution to a decision problem.

Table 3-2 Handwritten decision-making methods identified from the questionnaires

Method	Description
Mind Mapping	Visual brainstorming technique which creates a map like diagram. (Buzan & Buzan, 1996)
SWOT Analysis	Technique to identify strengths, weaknesses, opportunities and threats. (Fine, 2009)
Traffic Light System	Method to group information into level of difficulty: high (red), medium (amber) and low (green).
Scenario Analysis	Method to identify, implement, prioritize, and adapt market-driven business strategies. (Aaker, 2001)
Flowchart	Diagram that represents a process, displaying steps as shapes connected by arrows.
Kepner Tregoe Analysis	Management method for troubleshooting problems in four stages: situation analysis, problem analysis, decision analysis and problem/opportunity analysis. The decision analysis uses the needs and wants method for evaluation.
Decision Trees	Diagram that shows connected binary decisions and their outcomes.
Criteria Matrix/List	Brainstorming of decision criteria into either a list or matrix (table).
Pros, Cons and Uncertainties	Chart identifying advantages, disadvantages and the uncertainties present.
Risk, Rewards and Resources	Chart identifying uncertainties, outcomes and resource allocation.
Needs and Wants	Chart identifying the needs and wants of a company or individual.

3.3.1.2 Computational Decision-Making Methods

The respondents were asked about their use of computational decision-making methods. Thirty seven percent (37%) stated they did not use computer aided approaches, 21% use commercial software packages and 42% used Microsoft Excel. When asked to provide the names of the commercial software, the respondents cited Aspen HYSYS™ (http://www.aspentech.com), SciFinder™ (http://www.cas.org), HTRI™ Xchanger Suite (http://www.htri.net), STARLIMS™ (http://www.starlims.com) and Palisade @Risk (http://www.palisade.com).

The first four tools are able to locate physicochemical data which can represent decision variables but cannot be used to review and select decision alternatives.

Palisade @Risk, which was mentioned by one individual, has the capability to model risk and uncertainty within Microsoft Excel through the use of probability distributions. The respondents who used Microsoft Excel were asked in the questionnaire to describe how they utilised it. The majority used it to apply a simple additive approach (adding scores) or one of the simplest MCDA techniques, the Weighted Sum Method (WSM) (section 2.2.3.1). One of the respondents who described using the WSM in Excel said that the method was beneficial due to the straightforward nature of the calculations but they stated that the technique lacked support for modelling uncertainty.

3.3.2 Decisions made throughout WPD

While WPD considers the improvement of a whole process, from raw materials to end product, certain tasks in process design need to be considered in sequence. Sharratt (2011) proposed five stages for WPD (Table 3-3).

Table 3-3 Typical stages and decisions in Whole Process Design

Stage	Decisions at Stage
Route Selection	• Choice of chemical reactions for synthetic route. • Raw materials selection.
Process Concept	• Business needs and costing. • Batch or continuous. • Manufacture or acquisition.
Process Development	• Solvent selection. • Separation techniques. • Equipment requirements. • Compositions. • Conditions.
Flow Sheet Design	• Resource allocation. • Equipment selection.
Detailed Design	• Vessel and pipe selection. • Control method.

Generally the five stages are completed in succession. However, this will be project dependant as certain decisions may have to be fixed a-priori due to existing processing/product constraints. Nevertheless, at each WPD stage, Sharratt (2011) stated that a project "*might be terminated with a go/no go decision*" to essentially reduce costs by failing early. It was identified that 87.5% of the respondents use a gate system or project milestones to assess the proficiency of projects at each stage of process design.

The respondents were also asked to identify the decision problems that they regularly face. The most common decisions faced were associated with route selection (Figure 3-1). It is hypothesised that this may be due to projects being withdrawn before they reach the later stages of design or that decision-making in the later design stages is deemed to be less important with early stage decision-making being significant, in terms of the definition of the final process.

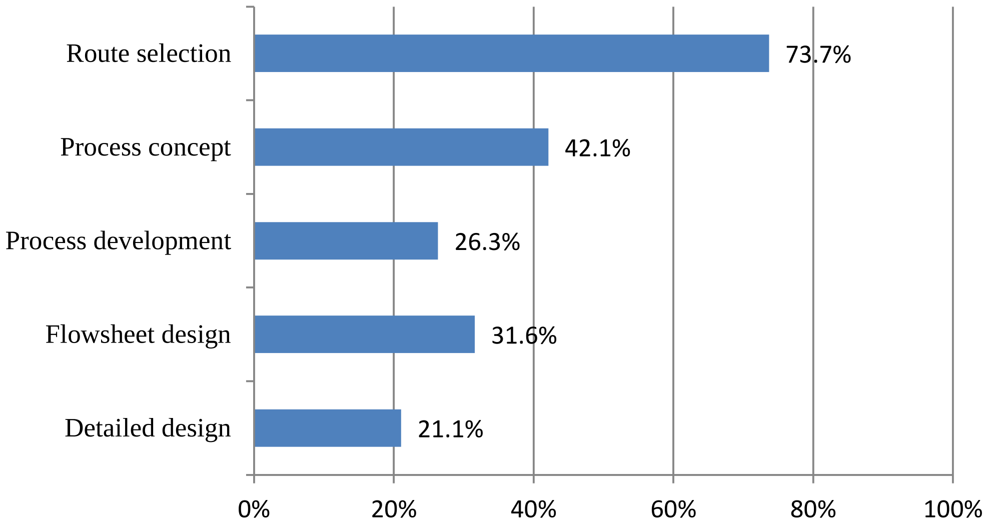


Figure 3-1 The percentage of respondents who face decisions at each stage of WPD

3.3.3 Requirements for a Decision-Making Framework

One question considered whether there was a need for a decision support tool to assist in the implementation of WPD. Ninety-five percent (95%) of the respondents confirmed that they would find a decision-making framework useful.

The remaining results in regard to the requirements for a decision-making framework are subdivided into sections relating to each phase of the decision-making process (see section 2.2.2.1). The first section investigates the industrial requirement for problem structuring. The second section investigates the requirement for a structured decision analysis. The final section addresses the responses related to the need for a post analysis study and issues pertaining to the design of a decision-making framework.

3.3.3.1 Problem Structuring

As discussed in section 2.2.2.1, the basis of problem structuring is to identify suitable criteria and alternatives for a decision problem. Only a quarter (26%) of the respondents said that they find it difficult to provide appropriate names for their criteria (i.e. to describe a measure that can be perceived by everyone in the company). However, over half (53%) of the respondents find it difficult to select a source to measure their criteria (for example, using the LD50 index to measure "Chemical Toxicity"). This could be due to the nature of the data available as all of the respondents said that their decisions were influenced by both qualitative and quantitative information.

With regards to identifying suitable alternatives (for example, chemical routes for a route selection problem), the respondents were asked if their decision problems comprised of a fixed number of alternatives or an infinite number of solutions. All respondents stated that they selected from a fixed number of alternatives with the majority (93%) selecting a small number of viable options from a larger collection of conceivable solutions. The remaining 7% of the respondents said they always make decisions from a small finite number of alternatives.

In terms of identifying criteria and alternatives, the respondents were asked if they preferred brainstorming by the use of a mind map or a list (e.g. pros and cons). Eighty six percent (86%) of the respondents favoured brainstorming via a list.

3.3.3.2 Decision Analysis

The need for a guidance tool as proposed by Robinon Brothers was investigated by asking whether the respondents would have favoured a system that produces exact results with a lengthy data entry procedure, or a system that guides the user in the right direction quickly. Eighty nine percent (89%) opted for the latter. This result clearly indicates the preference for a Multi-Attribute (MA) or outranking based approach as opposed to a Multi-Objective Optimisation (MOO) procedure.

The issue of the maximum time the respondents typically have available to analyse an important decision problem was considered. From Figure 3-2, 69% of the respondents would spend one hour or less analysing a decision problem. This renders a number of Multi-Criteria Decision Analysis (MCDA) techniques infeasible. For example, Doumpos and Zopounidis (2004) found that MCDA methods that require threshold values, such as ELECTRE and PROMETHEE, to be exceptionally time consuming to the extent of inhibiting real-world application. Likewise, Lootsma (1999) found MCDA methods which utilise pairwise comparisons, such as the Analytic Hierarchy Process, "*complicated and time-consuming*".

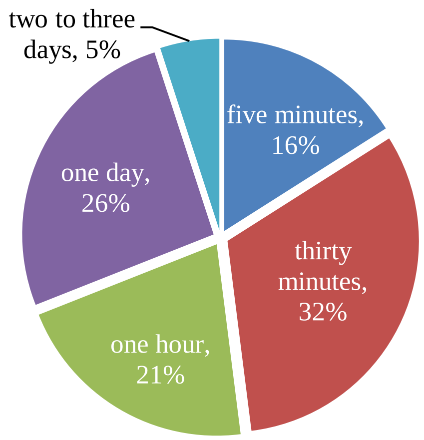


Figure 3-2 Maximum time the respondents have to solve a decision problem

Some MCDA methods require criteria to be represented by distributions, such as PROMETHEE. The respondents were asked if they would be comfortable selecting an appropriate distribution shape to define each of their criteria. As illustrated in Figure 3-3, the majority (67%) of the respondents indicated that they would only be able to select distributions under much guidance.

The respondents were also questioned regarding the inputs and outputs of a decision analysis. With regard to input, the respondents were asked which qualitative selection scale they would prefer from three options: small scale (1-5), medium scale (1-9) or large scale (1-100). Fifty three percent (53%) preferred small scale, 47% medium scale and 0% large scale.

With regard to output, the respondents were asked if they would prefer their results in the form of numerical values or a ranking. The results were inconclusive with 47% preferring numerical values and the remaining asking for a ranking.

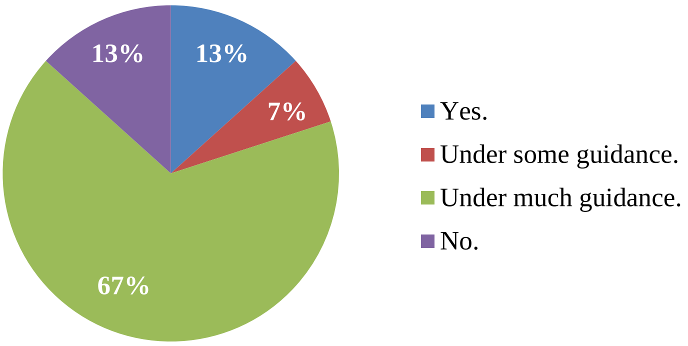
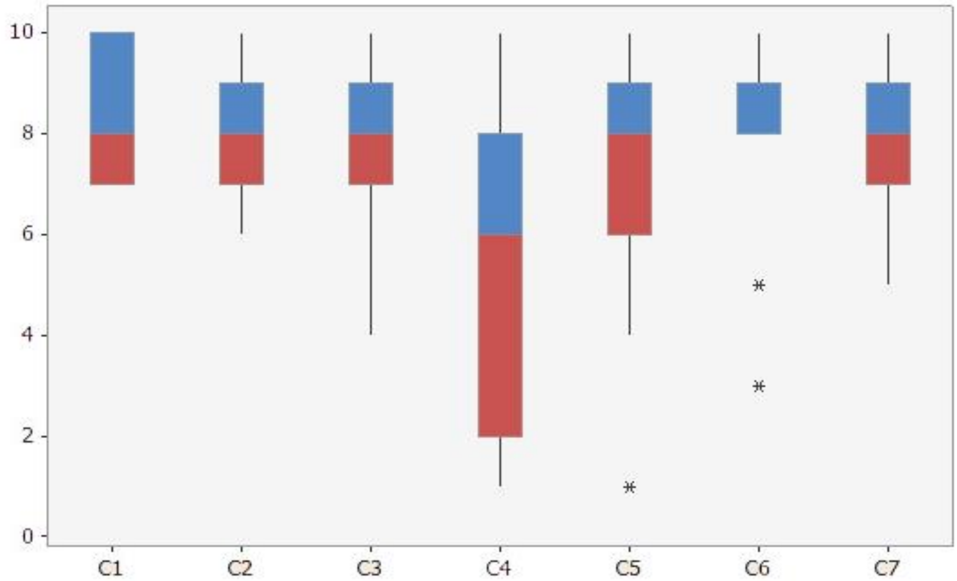


Figure 3-3 Percentage of respondents who feel comfortable using utility functions

3.3.3.3 Post Analysis and Design Features

The remaining series of questions focused on identifying the importance of design features, including the requirements for a post analysis study (see section 2.2.2.1). The respondents were asked to weight the importance of seven features on a scale of 1-10 (1 being extremely unimportant and 10 being extremely important). The results of the study are summarised in Figure 3-4. Five values can be identified from each plot, the lowest score, lower quartile (bottom of the red box), median (where red and blue meet), upper quartile (top of blue box) and the highest score. An asterisk represents an outlying score.



C1	Intuitive user interface	**C5**	Functionality for a sensitivity analysis
C2	Speed of operation and user input	**C6**	Support for group decision-making
C3	Influence from past decision-making or knowledge	**C7**	Functionality to record justification behind selections
C4	Compatibility with different operating systems		

Figure 3-4 Box plot of the importance of certain design features

C1 Intuitive user interface scored highly as the ease of operation is essential to ensure that the framework can be used rapidly and appropriately.

C2 Speed of operation and user input scored highly. This correlates with the responses shown in Figure 3-2.

C3 The high score for influence from past decision knowledge correlates with the results of the two interviews (section 3.2.3).

C4 The requirement for compatibility with different operating systems received a varied response. Compared to the other design features, C4 was the least preferred design feature by the respondents.

C5 Besides one outlier, the majority of the respondents favoured the capability of a sensitivity study in the post analysis phase of the decision process.

C6 Besides two outliers, the most sought after design feature was the ability to perform group decision-making. To confirm this, the respondents were also asked if they make decisions face-to-face in a group and/or need to consider external stakeholders (e.g. shareholders). Eighty seven percent (87%) of the respondents make decisions in a group environment and 80% need to consider external stakeholders.

C7 Functionality to record justification for each selection in a decision analysis scored highly. This feature allows for decision data to be stored for future decision-making. Therefore, this high score correlates with the requirement identified in the interviews to retrieve and reuse past decision knowledge.

3.4 Conclusions

The aim of this chapter was to address the following three research questions:

RQ4: What techniques are currently being used for decision-making in industry?

RQ5: What are the most common decisions made in WPD and in what stage of development are they considered?

RQ6: What does industry require from a decision-making framework?

Therefore the conclusions are presented in three sections, addressing each question in sequence.

3.4.1 Decision-making Techniques

From the mixed methods research conducted it is evident that few methods are utilised for a structured decision analysis in industry. Seventy eight percent (78%) of the respondents indicated that they use handwritten methods for decision-making. The majority of these methods are used to brainstorm a decision problem to identify suitable criteria and alternatives. None of the handwritten methods can be used to provide a solution for a decision problem. Twenty one percent (21%) of the respondents indicated that they use commercial software packages for decision-making. However, from asking the respondents to name the software tools, it was identified that none of them can be used to provide a solution for a decision problem. One package, @Risk, which was cited by one respondent, could be used to assist the modelling of uncertainty in a decision analysis using Microsoft Excel. Forty two percent (42%) of the respondents indicated that they use Microsoft Excel for decision-making. From further questioning it was identified that the two methods applied in Microsoft Excel were additive sum (adding weights) and the Weighted Sum Method (WSM). No other methods discussed in Chapter 2 were applied by the industrial members questioned.

3.4.2 Whole Process Design Decisions

From the WPD stages proposed by Sharratt (2011), the most cited decision problem was route selection. Route selection occurs predominently at the start of process design when there are high levels of uncertainty since there is limited understanding about the product and process. It can thus be concluded that industrial members require a decision-making tool that can handle uncertain information.

3.4.3 Framework Requirements

The work in this chapter has identified a number of industrial requirements for a decision-making framework. These are summarised in Table 3-4 as operational, design and functional specifications. Along with each specification a rationale is provided which describes or cites the justification for the specification.

In terms of operational requirements, professionals in the chemical-using industries require a system for rapidly making complex decisions with limited/uncertain information. Both quantitative and qualitative information must be considered to select between a finite numbers of alternatives. In terms of the design specification, the framework must be easy to use with at least one operating system. Users must be able to brainstorm their criteria and alternatives using lists and input their decision variables using a small to medium scale.

Table 3-4 Industrial Specification

	Operational Specification	Rationale
Result Accuracy	Moderate or better.	89% of the respondents favoured a system that guides the user in the right direction quickly over a system that produces exact results with a lengthy data entry procedure.
Modelling Time	1 hour or under.	69% of the respondents would spend one hour or less analysing a decision problem
Types of Input	Quantitative and Qualitative.	100% of the respondents said that their decisions were influenced by both qualitative and quantitative information.
Number of Alternatives	Finite	100% of the respondents said that they can identify a fixed number of alternatives to select from.
Uncertainty	Must handle Uncertainty.	See section 3.4.2.
	Design Specification	**Rationale**
Interface	Must be intuitive and easy to use.	See C1 in Figure 3-4.
Operating System	One or more platforms required.	See C4 in Figure 3-4.
Brainstorming Problem Input	List.	86% of the respondents favoured brainstorming via a list.
Analysis Input Scale	Small to Medium.	53% preferred a small input scale, 47% preferred a medium scale and 0% preferred a large scale.
	Functional Specification	**Rationale**
Required Functions	Ability to model Stage Gate™ decisions.	87.5% of the respondents use a gate system or project milestones.
	Recycle past decision knowledge.	Both interviewees require a framework that can retrieve and reuse past decision knowledge (see section 3.2.3).
	Problem Structuring Process.	See section 2.2.2.1.
	Sensitivity Analysis.	See C5 in Figure 3-4.
	Group Decision-Making.	87% of the respondents make decisions in a group environment.
	Stakeholder Analysis.	80% of the respondents need to consider external stakeholders.
	Record Justification/Rationality.	See C7 in Figure 3-4.

The framework must support stage gate decisions, sensitivity studies, group decision-making and stakeholder analyses. Furthermore, the framework must incorporate a problem structuring process, be able to utilise past decision knowledge and record rationality for each of the users' selections.

The following chapter uses the information presented in this chapter and chapter 2 to addresses the overarching research question of this thesis:

RQ1: What is the most effective way to support decision-making in whole process design?

Following this, a methodology is proposed along with a decision-making framework to validate the proposed methodology.

"A picture is worth a thousand words. An interface is worth a thousand pictures."

Ben Shneiderman (2003)

4 Materials and Methods

4.1 Introduction

The review of decision-making methods in chapter 2 and the identification of industrial requirements in chapter 3 enable RQ1 to be addressed:

RQ1: What is the most effective way to support decision-making in whole process design?

A solution to RQ1 is proposed at the start of this chapter along with a methodology. To validate the proposed methodology, the proceeding section introduces a decision-making framework that incorporates two other commonly applied decision-making methods.

4.2 Decision-Making in Whole Process Design

It was identified in Table 3-4 that professionals in the chemical-using industries require a solution for rapidly making complex decisions with limited/uncertain information. Additionally, the solution must consider both quantitative and qualitative information to select between a small/finite number of alternatives. The benchmark study of decision-making methods in Table 2-1 shows that Multi-Objective Optimisation (MOO) methods use quantitative information to search an infinite number of alternatives. They have a high modelling time and cannot handle uncertainty as well as MA and outranking methods. MA and outranking methods on the other hand use both qualitative and quantitative information to evaluate a finite number of alternatives. They also have a low modelling time in comparison to MOO methods. Therefore, the attributes of MA and outranking methods outperform MOO methods in respect to the requirements of the industrial professionals (Table 3-4). However, there are a range of techniques that are available within these two method families (section 2.2.4 and 2.2.5).

The literature review focusing on chemical engineering (section 2.4.2) identified three MA methods that have previously been applied to decision-making within product and process design; Analytic Hierarchy Process (AHP), Analytic Network Process (ANP) and Weighted Sum Method (WSM). The questionnaires (section 3.3.1) revealed that out of these three methods, the industrial members of Britest only utilised WSM using Microsoft Excel.

The main issue with applying WSM to assist in the decision-making process in Whole Process Design (WPD) is that the method is unable to handle uncertain information. Section 2.3.3 summarised a range of methods to account for uncertainty in MA and outranking methods. One approach proposed was through the application of a sensitivity analysis. George et al. (2007) proposed a variation of the WSM that incorporates a global sensitivity analysis using Monte Carlo simulation. A global sensitivity analysis differs from a 'one-at-a-time' sensitivity study with all the decision variables being changed. George et al. (2007) stated that "*the WSM proved to be highly suitable for data handling and for the analysis of results*". However, the Monte Carlo simulations require many iterations to understand the sensitivity of a model and due to the different starting values of the algorithm, the results are not repeatable.

Multi-Attribute Range Evaluations (MARE) is proposed as a novel approach to the WSM that uses one iteration to visually convey the decision results with associated levels of uncertainty.

4.3 Multi-Attribute Range Evaluations

Multi-Attribute Range Evaluations (MARE) is a novel approach that utilises the Weighted Sum Method (WSM). The WSM calculates a score for each alternative, A_i by summing the products of each decision variable (a_{ij}) and its corresponding criterion weight (w_j), as given in equation 2-7:

$$A_i = \sum_{j=1}^{n} w_j a_{ij} \qquad for\ i = 1,2,\dots,m. \tag{2-7}$$

where a decision problem has m fixed alternatives and n fixed criteria. a_{ij} is the decision variable for the i^{th} alternative with respect to the j^{th} criterion.

The decision-maker can provide values (b_j) for the importance of each criterion or directly provide criteria weights (w_j) that sum to one. If values are provided, the summation ratio normalisation method (equation 4-1) is used to convert the values into weights:

$$w_j = \frac{b_j}{\sum_{j=1}^{n} b_j} \qquad \textbf{4-1}$$

where a decision problem has n fixed criteria, b_j denotes the criterion value of the j^{th} criterion and w_j denotes the criterion weight of the j^{th} criterion.

The MARE methodology supports both limited knowledge and uncertain selections by allowing more than one value to be allocated to each decision variable (a_{ij}). The decision-maker can assign up to three values for each alternative (A_j) in terms of each criterion (C_j). These values represent the most likely value (a_{ij}), the minimum possible value (a_{ij}^{min}) and the maximum possible value (a_{ij}^{max}). If the decision variable is certain and no values are provided for a_{ij}^{min} or a_{ij}^{max}, a_{ij} is used for all three values.

Quantitative information is required in the form of numerical values. Qualitative information must be provided as subjective scores within a comparable range: for example, 1-10. If MARE is applied as a software tool, slider bars (Figure 4-1a) can be utilised for qualitative input rather than numerical entry as they provide the decision-maker with a visual representation of their selections. Furthermore, a range slider bar can allow for rapid entry of three inputs with no data validation required (i.e. $a_{ij}^{min} \leq a_{ij} \leq a_{ij}^{max}$). Figure 4-1b illustrates a range slider bar where the slider for a_{ij} is positioned within a darkened range. The starting position (at the left) of the darkened range represents the value of a_{ij}^{min} and the end position (at the right) represents the value of a_{ij}^{max}. As presented, qualitative word models can be used to describe the position of a_{ij} within a selection panel (for example: poor, average, good etc.).

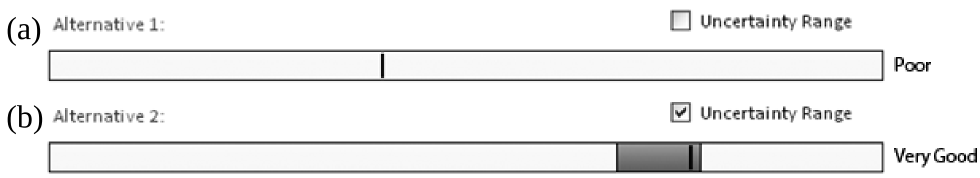


Figure 4-1 Qualitative input for the MARE Method

The WSM is currently incapable of combining multidimensional data and consequently different measurement units (Pohekar & Ramachandran, 2004). A proposed solution is to normalise the decision variables (a_{ij}). As the transformation needs to have an equal scale length for the minimum, likely and maximum values, a normalisation procedure that divides by the sum of all the decision variables cannot be applied. Therefore, the max scale normalisation procedure (Chakraborty & Yeh, 2007) that utilises the largest decision variable (a_j^{max}) for normalisation is used:

$$a_{ij} = \frac{a_{ij}}{a_j^{max}} \qquad {a_{ij}}^{min} = \frac{{a_{ij}}^{min}}{a_j^{max}} \qquad {a_{ij}}^{max} = \frac{{a_{ij}}^{max}}{a_j^{max}} \tag{4-2}$$

This procedure is applied to all the decision variables resulting in a value between 0 and 1. Equation 2-7 is then used to calculate the scores for each of the alternatives with respect to the minimum, most likely and maximum. The scores are represented by a value between 0 and 1, with the scores closer to 1 being superior alternatives. The results can be visualised by plotting the most likely score with high/low lines, as shown in Figure 4-2. The length of the high/low lines represents the uncertainty associated with a particular alternative, i.e. a short high/low line represents a greater level of certainty than one with a long high/low line.

Considering the example in Figure 4-2, it can be seen that Alternative 2 is marginally better than Alternative 1 and Alternative 4 in terms of the most likely value. However, the decision-maker may wish to select Alternative 4 as there is less uncertainty associated with this option.

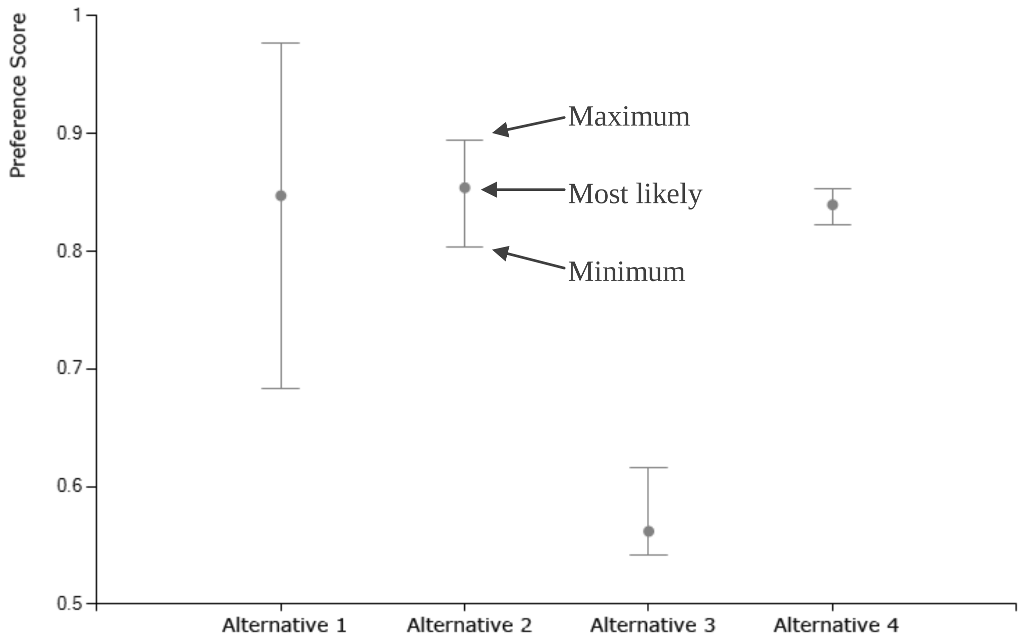


Figure 4-2 A hypothetical output of the MARE methodology

4.4 Evaluation Strategy

The MARE methodology was proposed to extend the WSM approach that industry had previously applied. MARE takes into account imprecise and uncertain preferences that are typically present at the early stages of WPD. The ability to visualise uncertainty provides the MARE approach with a number of advantages over other MCDA methods. However, other MA and outranking approaches also have unique advantages. Therefore, this chapter will present a framework, ChemDecide, that incorporates MARE and two other decision analysis methods to be compared. The two methods selected were Analytic Hierarchy Process (AHP) and ELECTRE III as the literature suggests that these are the best approaches from the methodological fields of MA (see section 2.2.4.4) and outranking (see section 2.2.5.4) respectively. Table 4-1 shows a comparison of the three methods including the advantages and limitations of each.

As discussed in section 2.2.1, Huang et al (2011) believes that the widespread use of AHP is related to the availability of user-friendly and commercially supported software packages. To remove any biases in the study, the three analysis tools were developed utilising identical controls (e.g. text boxes, slider bars and click buttons) and forms (application windows) where possible. The Graphical User Interface (GUI) is presented and discussed in Appendix B.

The three analysis tools were evaluated using real-world industrial case studies carried out by professionals working in the chemical-using industries. Three independent decision case studies are discussed in Chapter 5, with the aim of identifying the capability of each analysis tool for addressing WPD decision problems.

4.5 ChemDecide Framework

The following section provides an overview of the ChemDecide Framework followed by a more detailed description of each tool incorporated within the framework. An implementation plan is finally discussed relating to the interface design that is presented in Appendix B.

Table 4-1 Comparison of the analysis methods in the ChemDecide Framework

	AHP	MARE	ELECTRE III (RANK)
Method Summary	1. Decision problem modelled in a hierarchy. 2. Pairwise comparisons are used for qualitative measurement. 3. Scores are provided by eigenvector calculations.	1. Minimum, most likely and maximum scores can be used for measurement. 2. Scores aggregated using weighted sum method. 3. Uncertainty can be visualised.	1. Thresholds used to calculate pairwise comparisons of alternatives. 2. Positive and negative aspects of each alternative creates credibility index. 3. Ranking calculated.
Input	Quantitative scores, pairwise comparisons.	Qualitative and Quantitative scores, weights.	Qualitative and Quantitative scores, thresholds, weights.
Output	Cardinal scores	Cardinal scores	Ordinal rank
Decision-Maker Interaction[a]	High	Moderate	Moderate
Uncertainty	Not considered directly[b]	Visualised in output	Fuzzy (pseudo-criteria)
Strengths	1. Pairwise comparisons provide an uncomplicated way to enter qualitative preferences.	1. Algorithm is relatively straightforward to use. 2. Output provides high amounts of information.	1. Very poor performance on a single criterion may eliminate an alternative from consideration[c].
Limitations	1. Possibility for intransitive preferences. 2. High number of pairwise comparisons required for large scale problems.	1. Further decisions may have to be considered upon reviewing the output.	1. Algorithm used is relatively complex and may not be understood by the decision-maker. 2. A complete ranking of the alternatives may not be achieved.

[a] from Malczewski (1999)

[b] from Millet & Wedley (2003)

[c] from Linkov et al. (2006)

4.5.1 Framework Overview

The ChemDecide framework consists of four modules, one related to problem structuring and the other three are associated with the analysis (Figure 4-3). The problem structuring tool is termed Decision Structure. The analysis tools AHP and MARE are known by their respective methodological names while ELECTRE III has been shortened to RANK. The rationale for developing an independent problem structuring tool was a consequence of the following:

- Problem structuring is often overlooked in a decision-making process (section 2.2.2.1) and by having a separate tool to guide the user through this phase forces them to consider their selections in a detailed yet structured manor.
- As discussed in section 2.2.4.2, AHP suffers from rank reversals. Prohibiting the user from adding or removing alternatives and criteria from the decision model ensures rank reversals cannot occur.
- Separating the problem structuring phase from the decision-making procedure will ensure the decision problem remains consistent throughout all three analyses. Hence, comparative results will be attained from the industrial evaluations and the conclusions drawn.

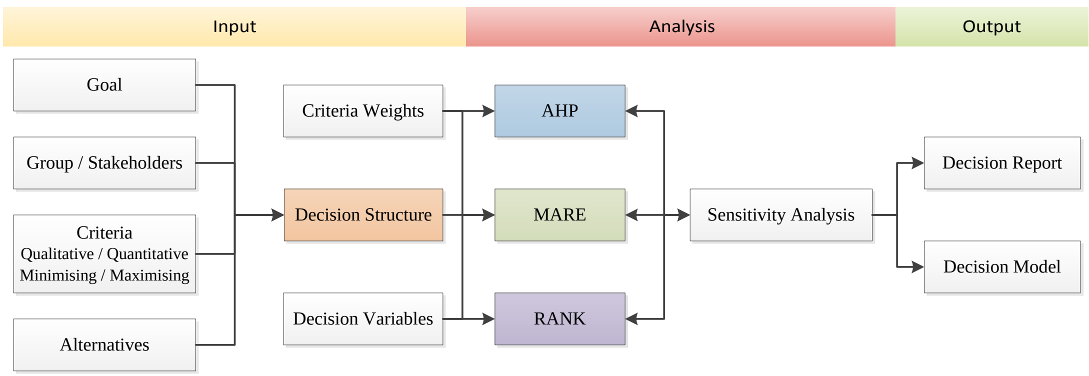


Figure 4-3 Overview of the ChemDecide Framework

As shown in Figure 4-3, the problem structuring tool requires the decision-maker(s) to define a goal, a set of alternatives and a defined set of criteria (including if each criterion is qualitative/quantitative and minimising/maximising). Decision Structure compiles this information into a single file which can be accessed by any of the three analysis tools. The analysis tools, which calculate a decision result, require the decision-maker(s) to input criteria weights and decision variables along with the rationale for each selection. These inputs can be altered to investigate the sensitivity of the results. Once a decision outcome is accepted, the analysis tools can compile all of the decision information into a single file (model) or generate a report containing the results.

The ChemDecide framework was developed using C# in Microsoft Visual Studio 2010 and .NET Framework 4.0. This approach was adopted for the following reasons:

- The ChemDecide framework can be installed and executed as a standalone software without the requirement for external software packages, thereby encouraging industrial members to evaluate the software.
- The .NET framework provides a range of libraries for input/output controls and data visualisation charts which could be incorporated into the ChemDecide GUI.
- There are many external libraries available online that have free licences for mathematical and algorithmic support.

The only limitation of C# and .NET is that the ChemDecide framework can only be compiled for use on a Windows based operating system.

4.5.2 Logical Overview

This section presents a more detailed discussion of each of the four tools in the ChemDecide Framework.

4.5.2.1 Decision Structure

Decision Structure is the tool that helps the decision-maker to structure their problem. The goal is to guide the user through the selection and verification of a feasible set of alternatives and criteria. The whole process should be sufficiently flexible to allow for changes as the decision-maker becomes more immersed in the problem (see section 2.2.2.1). Figure 4-4 provides a flow diagram of the process utilised in Decision Structure and the iterative procedure that is built-in to ensure that the decision-maker identifies appropriate criteria and alternative sets.

Firstly, the decision-maker must identify the decision goal, record the team membership and schedule a deadline for the completion of the analysis. The decision-makers can then brainstorm whist considering external stakeholders to attain a perspective of the views and objectives of thedecision problem. Although this information is not used directly in the analysis, the procedure focuses the users thought process on the problem and potential associated issues. The next stage is to determine the decision alternatives followed by their related criteria. To aid in the selection of the criteria, the values and objectives discussed during the brainstorming section can be reviewed. Along with a criterion name, the decision-maker must identify if it is qualitative or quantitative (criteria source) and whether it is to be minimising or maximising (aim). The team can then define the criteria in more detail by recording a description of why each criterion is essential and provide a data source. This information is useful if the decision-maker wants to return to the decision analysis in the future or generate an analysis report.

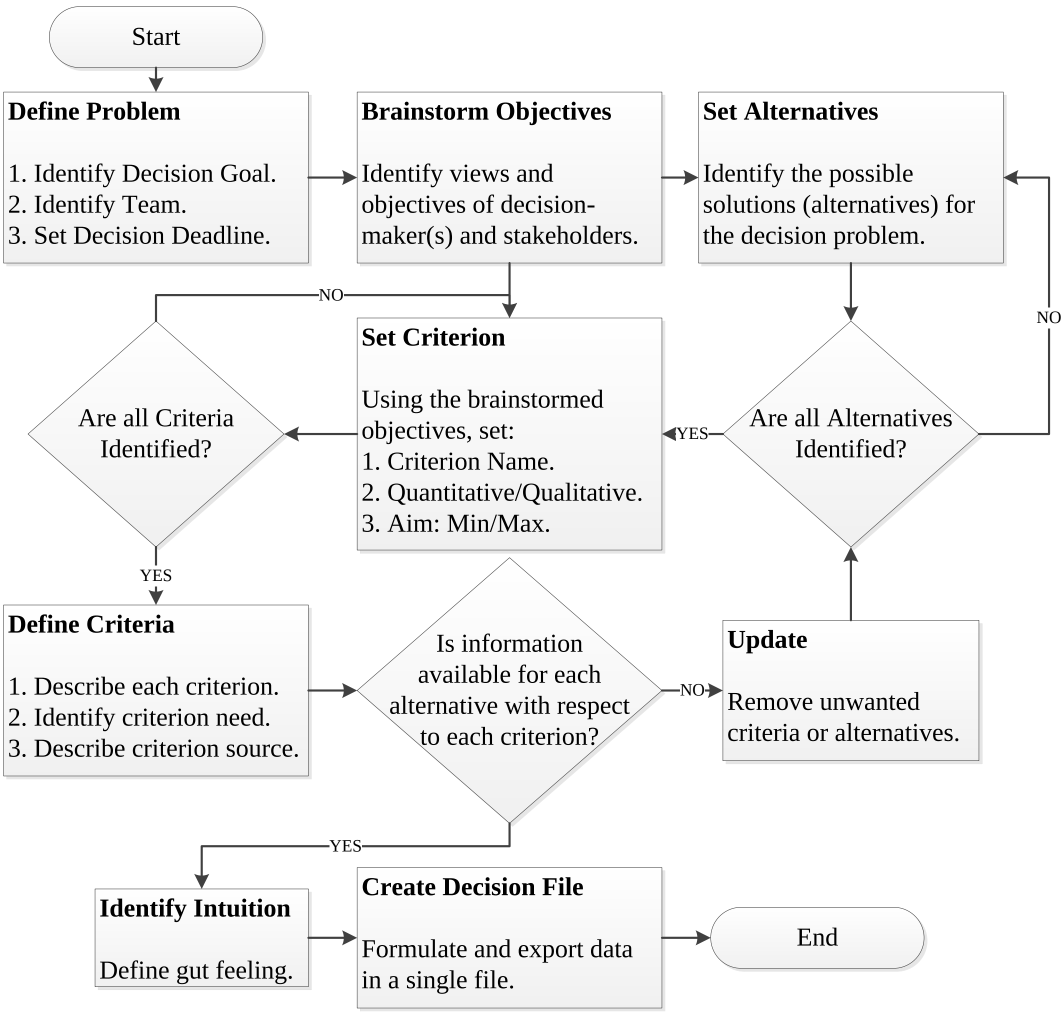


Figure 4-4 Decision Structure Logical Overview

The final task, which is critical to the analysis, requires the team to review the criteria and alternatives to ensure that it is possible to represent each decision variable by a numerical value or a subjective score. If the team cannot source representation, the decision-maker can return to a previous part of the procedure to update the criteria and alternative sets. If the review is successful, the team can identify an alternative to represent their intuition (gut feeling) and complete the decision structuring process.

The Decision Structure module can create a decision file which contains all of the information collated during the problem structuring process and is available for analysis by each of the decision analysis modules.

4.5.2.2 Analytic Hierarchy Process (AHP)

The AHP module guides the decision-maker through the Analytical Hierarchy Process (Saaty, 1972, 1980). The workflow for this process is given in Figure 4-5. Firstly the decision-maker opens a file created in Decision Structure which contains the criteria and alternatives for the decision problem. The user then pairwise compares the criteria and the values are placed into a reciprocal matrix (section 2.2.4.2). The matrix is used to calculate the principle eigenvectors which represent the criteria weights. The method selected to calculate the principle eigenvectors was the technique utilised by Saaty (1980) as shown in the three steps below:

1. Multiply the elements within each row of a matrix.

	a1	a2	a3	a4	Multiplied Rows
a1	1	1/4	4	1/6	= 0.1666
a2	4	1	4	1/4	= 4
a3	1/4	1/4	1	1/5	= 0.0125
a4	6	4	5	1	= 120

2. For each row, take the nth root of the multiplied product.

Multiplied Rows	Nth Root
$0.1666^{(1/4)}$	= 0.638943
$4^{(1/4)}$	= 1.414214
$0.0125^{(1/4)}$	= 0.33437
$120^{(1/4)}$	= 3.309751
Sum:	= 5.697278

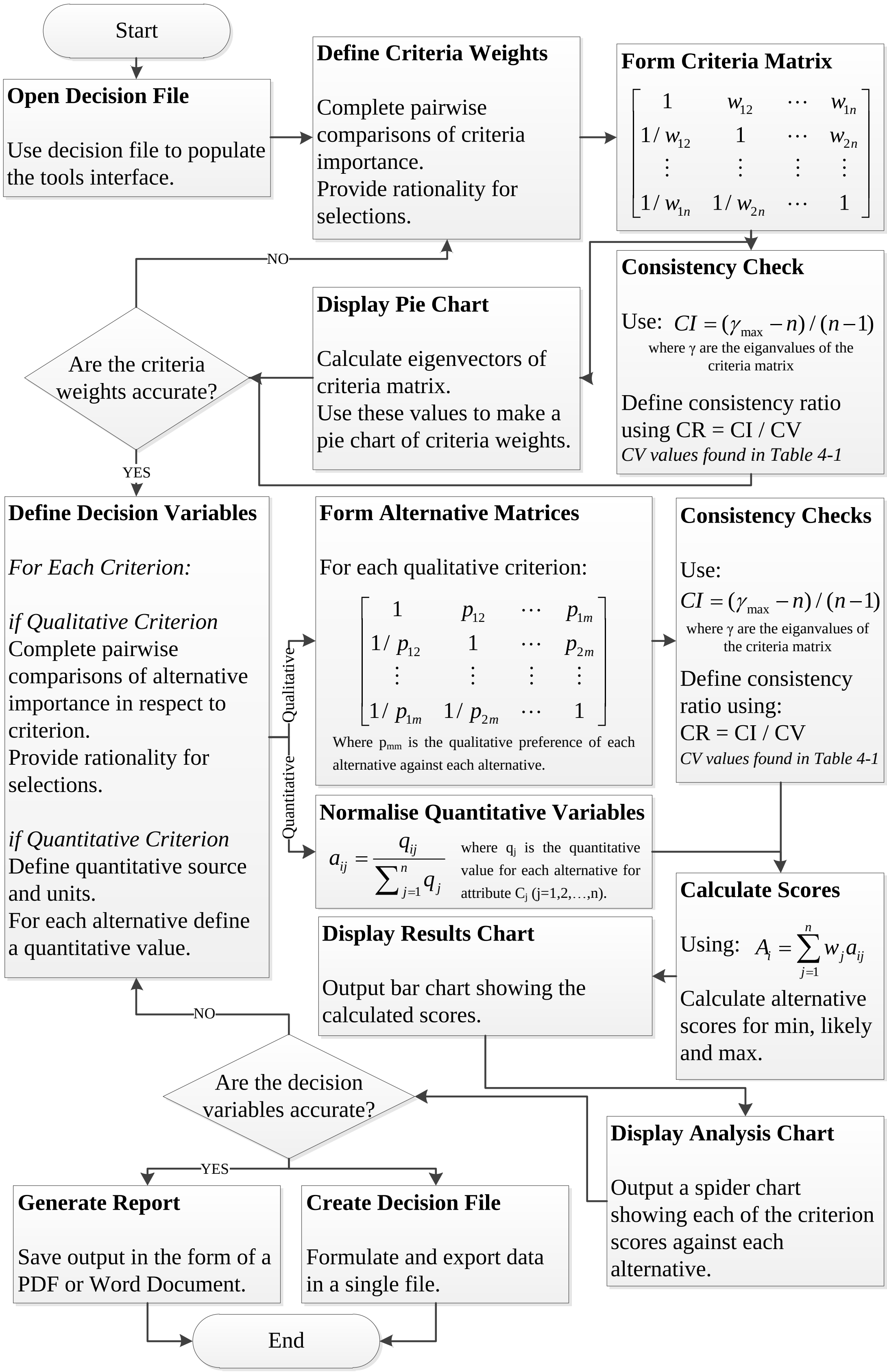


Figure 4-5 AHP Logical Overview

3. Normalise the nth root values by dividing by the sum.

Nth Root	**Priorities**
0.638943	= 0.112149
1.414214	= 0.248226
0.33437	= 0.058689
3.309751	= 0.580936

A consistency check is used to ensure the decision-maker has not violated transitivity (section 2.2.4). The consistency check uses Consistency Values (CV) derived from random judgements (Table 4-2) in a four step process outlined below.

Table 4-2 Consistency Values (Saaty, 1980)

n	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
CV	0	0	0.58	0.9	1.12	1.24	1.32	1.41	1.45	1.49	1.51	1.48	1.56	1.57	1.59

1. Sum the elements in each column and multiply by the principle eigenvectors.

	a1	**a2**	**a3**	**a4**	**Priorities**
a1	1	1/4	4	1/6	0.112149
a2	4	1	4	1/4	0.248226
a3	1/4	1/4	1	1/5	0.058689
a4	6	4	5	1	0.580936
Sum:	11.25	5.5	14	1.616667	
Sum*Priority:	1.261676	1.365243	0.821646	0.93918	

2. Calculate $\gamma_{\max}$ by summing the calculated values.

					$\gamma_{\max}$
Sum*Priority:	1.261676	1.365243	0.821646	0.93918	= 4.387745

3. Calculate the Consistency Index using: $CI = (\gamma_{\max} - n)/(n-1)$

   $(4.387745 - 4) / (4 - 1) = 0.129248$

4. Calculate the Consistency Ratio using: CR = CI / CV

   0.129248 / 0.9 (taken from Table 4-2) = 0.143609

   This value suggests that the pairwise comparisons are inconsistent.

Saaty (1980) suggested that a CR of 0 infers perfect consistency while a CR above 0.1 is considered inconsistent. Bearing in mind the values in Table 4-2 are derived from randomly generated judgements, the 0.1 threshold for inconsistency is considered very strict and impractical. Therefore, the AHP tool notifies the decision-maker for borderline inconsistency when CR is between 0.8 and 0.125 and caution for absolute inconsistency when CR is above 0.125. When warned, the decision-maker can examine their pairwise comparisons for errors and amend their selections.

After the criteria weights are established, the decision-maker needs to define appropriate decision variables. The decision variables in respect to the qualitative criterion are provided as pairwise comparisons and are calculated in the same way as the criteria weights. The decision variables in respect to the quantitative criteria are provided as numerical scores and are normalised using the equation in Figure 4-5.

Final scores are calculated using the WSM, given in equation 2-7. The results are shown along with an analysis chart that presents the decision variables on a spider diagram (see Appendix B). The user can conduct a sensitivity analysis by modifying the criteria weights and/or decision variables. On completion, a report can be generated or a decision file containing all the decision-makers' preferences can be exported.

4.5.2.3 MARE

The MARE tool guides the decision-maker through the process explained in section 4.3. The relevant workflow is shown in Figure 4-6. Initially, the decision-maker opens a file created in Decision Structure which contains the criteria and alternatives for the decision problem. Subsequently, the decision-maker must define the criteria weights using a slider bar for each criterion. These weights are normalised using equation 4-1. The decision-maker must then define the decision variables. For decision variables in respect to qualitative criterion, slider bars (single selection) are used for input that is certain and range slider bars (three selections) are used for uncertain input. For decision variables in respect to quantitative criterion, numerical values are required, one if certain and three if uncertain. Final scores are calculated using equation 2-7 and the decision results are shown along with an analysis chart that shows the most likely decision variables. A sensitivity study can be conducted, a report can be generated or a file containing the decision information can be saved.

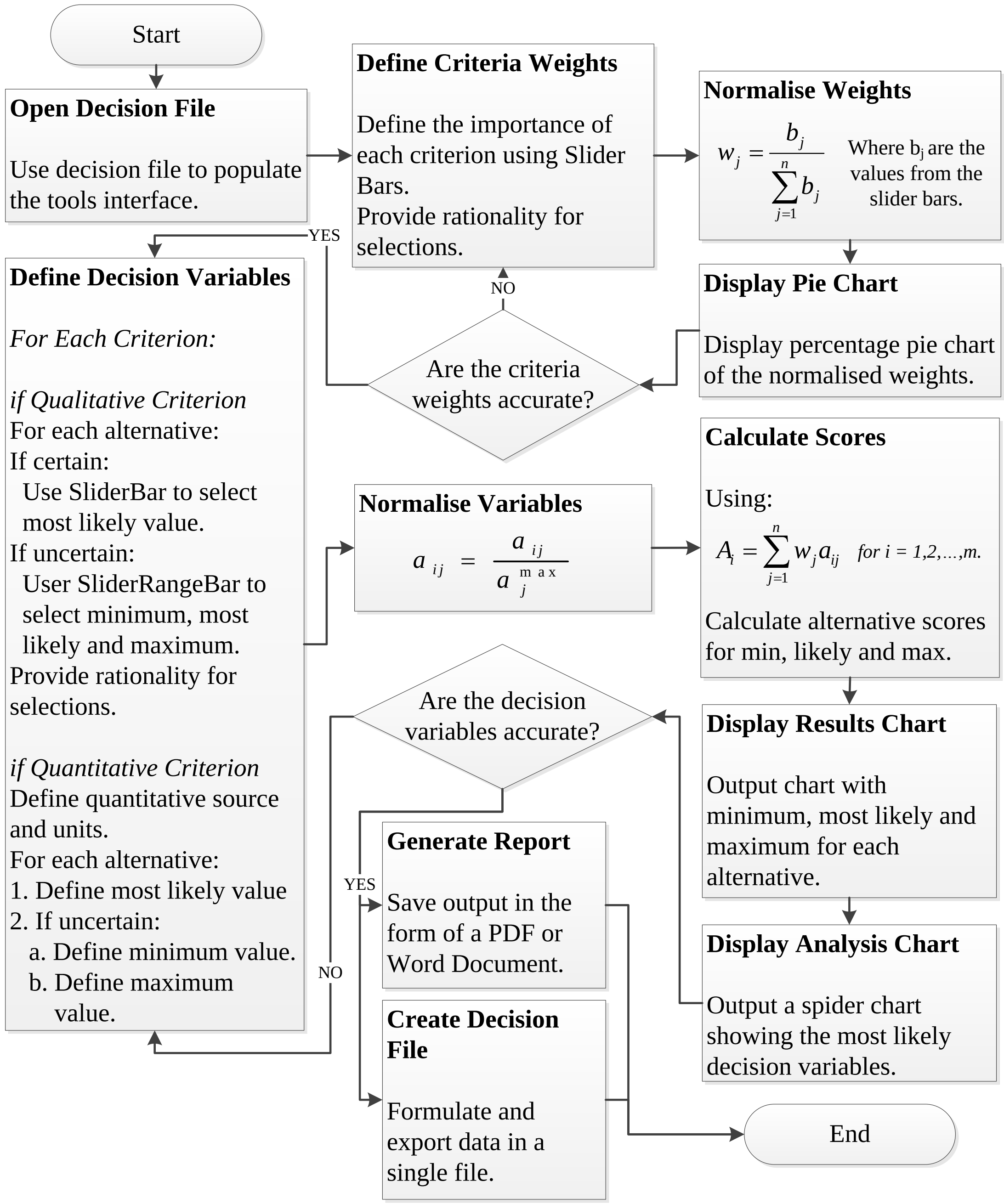


Figure 4-6 MARE Logical Overview

4.5.2.4 RANK

The RANK tool guides the decision-maker through the ELECTRE III method (section 2.2.5.1). The workflow of the RANK tool is shown in Figure 4-7. After the criteria and alternatives are extracted from the Decision Structure file, the decision-maker must define the criteria weights. This is accomplished in an identical way to the MARE module by using slider bars and the normalisation procedure in equation 4-1.

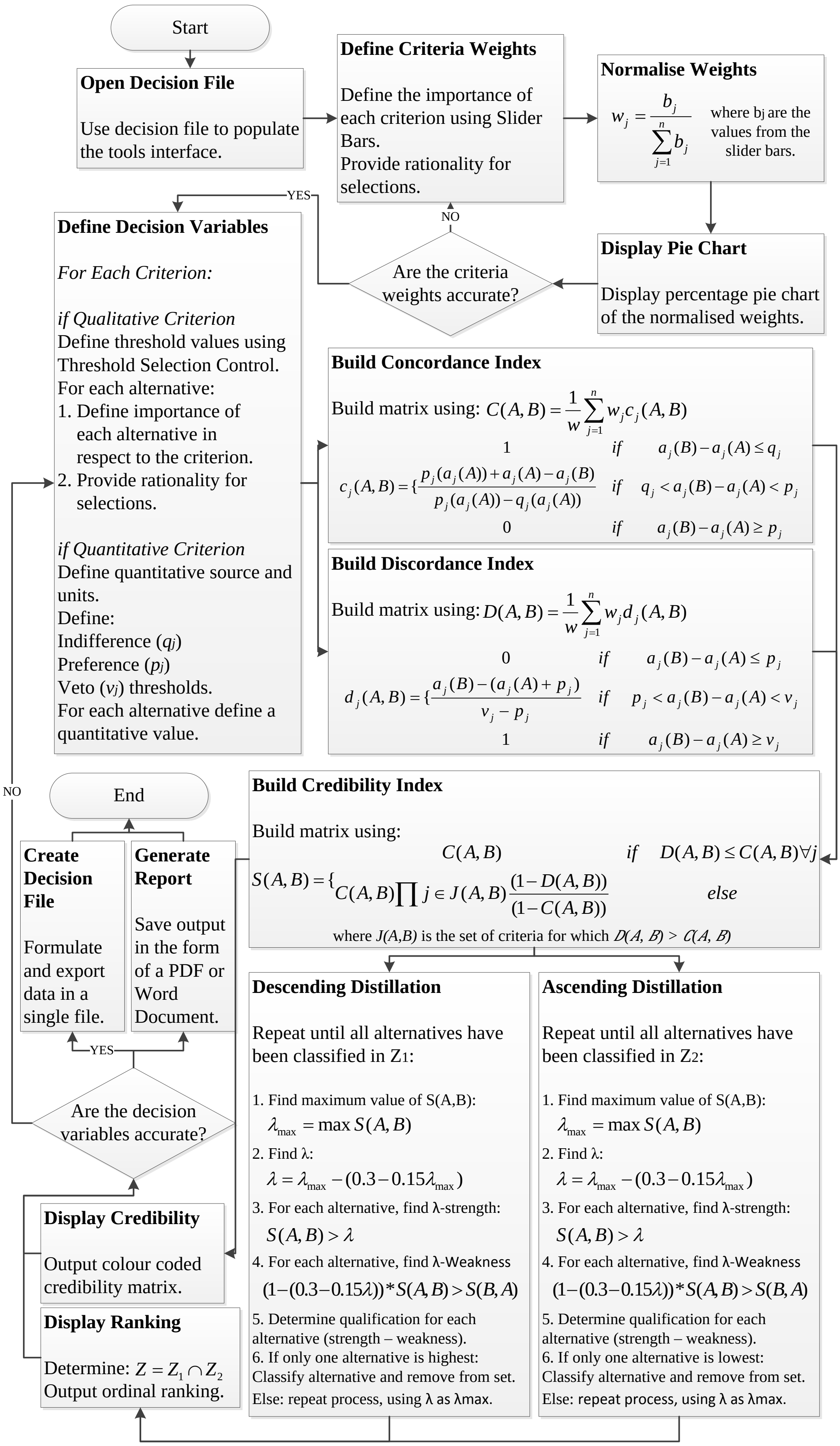


Figure 4-7 RANK Logical Overview

The decision-maker must then define decision variables and threshold values. Decision variables in respect to qualitative criteria are input with slider bars and decision variables in respect to quantitative criteria are input as numerical values. Similarly, threshold values in respect to qualitative criteria are input with a threshold selection slider bar (section 4.5.3) and threshold values in respect to quantitative criteria are input as numerical values. Three threshold values are required for each criterion: indifference (q_j), preference (p_j) and veto (v_j). The threshold values are used to build concordance and discordance indices using equations 4-3 and 4-4 respectively.

$$C(A,B) = \frac{1}{w}\sum_{j=1}^{n} w_j c_j(A,B) \quad \textit{using:}$$

$$c_j(A,B) = \begin{cases} 1 & \textit{if} \quad a_j(B) - a_j(A) \le q_j \\ \dfrac{p_j(a_j(A)) + a_j(A) - a_j(B)}{p_j(a_j(A)) - q_j(a_j(A))} & \textit{if} \quad q_j < a_j(B) - a_j(A) < p_j \\ 0 & \textit{if} \quad a_j(B) - a_j(A) \ge p_j \end{cases} \qquad \textbf{4-3}$$

where A and B are decision variables, n is the number of criteria, w_j is the weight of criterion j, q_j is the indifference threshold for the criterion j and p_j is the preference threshold for the criterion j.

$$D(A,B) = \frac{1}{w}\sum_{j=1}^{n} w_j d_j(A,B) \quad \textit{using:}$$

$$d_j(A,B) = \begin{cases} 0 & \textit{if} \quad a_j(B) - a_j(A) \le p_j \\ \dfrac{a_j(B) - (a_j(A) + p_j)}{v_j - p_j} & \textit{if} \quad p_j < a_j(B) - a_j(A) < v_j \\ 1 & \textit{if} \quad a_j(B) - a_j(A) \ge v_j \end{cases} \qquad \textbf{4-4}$$

where A and B are decision variables, n is the number of criteria, w_j is the weight of criterion j, p_j is the preference threshold for the criterion j and v_j is the veto threshold for the criterion j.

A worked example, adapted from Buchanan et al. (1999), showing the calculations to form a concordance and discordance index is shown below.

Considering a 5 criteria (c1,c2,..,c5) and 5 alternative (a1,a2,..,a5) problem:

	c1	**c2**	**c3**	**c4**	**c5**
a1	-14	90	0	40	100
a2	129	100	0	0	0
a3	-10	50	0	10	100
a4	44	90	0	5	20
a5	-14	100	0	20	40
indifference (q_j)	25	16	0	12	10
preference (p_j)	50	24	1	24	20
veto (v_j)	100	60	2	48	90
weight (w_j)	1	1	1	1	1

The concordance calculations for alternatives a1 and a5 are:

c1(a2,a5) = 1, as $-14-129 \leq 25$

c2(a2,a5) = 1, as $100-100 \leq 16$

c3(a2,a5) = 1, as $0-0 \leq 0$

c4(a2,a5) = $\frac{24+0-20}{24-12}$ = 0.333, as $12 < 20-0 < 24$

c5(a2,a5) = 0, as $40-0 \geq 20$

Therefore, C(a2,a5) = $\frac{(1)(1)+(1)(1)+(1)(1)+(1)(0.333)+(1)(0)}{1+1+1+1+1}$ = 0.66667

The discordance index for alternative a1 and a2 is:

D(a1,a2) = 1, as in terms of c1: $129 - (-14) \geq 100$

The calculations are performed on every pair of alternatives to build a concordance matrix and discordance matrix. These matrices are used to calculate a credibility index using:

$$S(A,B) = \begin{cases} C(A,B) & \text{if} \quad D(A,B) \leq C(A,B) \forall j \\ C(A,B) \prod j \in J(A,B) \dfrac{(1-D(A,B))}{(1-C(A,B))} & \text{else} \end{cases} \qquad \textbf{4-5}$$

where *J(A,B)* is the set of criteria for which *D(A, B)* > *C(A, B)*

The calculation assumes that if the strength of the concordance index exceeds that of the discordance index then the concordance value should not be altered. If the discordance index exceeds that of the concordance index, the value needs to be modified.

The credibility matrix assesses the strength of the assertion that *A* is at least as good as *B* and is used to determine a ranking of the alternatives. The ranking is calculated through two distillations, a descending distillation (*Z1*) and an ascending distillation (*Z2*) shown in Figure 4-8. The 0.3 and 0.15 values used in step 2 were recommended by Roy and Bouyssou (1993).

Descending Distillation

Repeat until all alternatives have been classified in Z1:

1. Find maximum value of S(A,B) using:
   $\lambda_{\max} = \max S(A, B)$
2. Find λ using:
   $\lambda = \lambda_{\max} - (0.3 - 0.15\lambda_{\max})$
3. For each alternative, find λ-strength using:
   $S(A, B) > \lambda$
4. For each alternative, find λ-Weakness using:
   $(1 - (0.3 - 0.15\lambda)) * S(A, B) > S(B, A)$
5. Determine qualification for each alternative (strength – weakness).
6. If only one alternative is highest:
   Classify alternative and remove from set.
   Else: repeat process, using λ as λmax.

Ascending Distillation

Repeat until all alternatives have been classified in Z2:

1. Find maximum value of S(A,B) using:
   $\lambda_{\max} = \max S(A, B)$
2. Find λ using:
   $\lambda = \lambda_{\max} - (0.3 - 0.15\lambda_{\max})$
3. For each alternative, find λ-strength using:
   $S(A, B) > \lambda$
4. For each alternative, find λ-Weakness using:
   $(1 - (0.3 - 0.15\lambda)) * S(A, B) > S(B, A)$
5. Determine qualification for each alternative (strength – weakness).
6. If only one alternative is lowest:
   Classify alternative and remove from set.
   Else: repeat process, using λ as λmax.

Figure 4-8 Descending and Ascending Distillation Algorithms

The descending distillation classifies the alternatives with the highest qualification first while the ascending distillation classifies the alternatives with the lowest qualification first. The final order (*Z*) is obtained through combining *Z1* and *Z2*. This is achieved by aggregating the two distillations into a ranking matrix. If *A* is ranked higher than *B* in both distillations, or *A* is better than *B* in one distillation and has the same ranking in the other distillation *Z(A,B)* = 1, otherwise *Z(A,B)* = 0. Summing the rows of the ranking matrix gives scores for each alternative. The alternative with the highest score is ranked first and the alternative with the lowest score receives the worst rank. If two or more alternatives have the same score then then they are classified in the same rank position. A worked example, modified from Giannoulis and Ishizaka (2010), is presented below using the following *Z1* and *Z2* distillations:

RANK:	**1**	**2**	**3**	**4**	**5**	**6**
Z1:	a5	a1, a3		a2	a6	a4
Z2:	a2, a5		a1, a3		a6	a4

The ranking matrix for the 6 alternatives (a1,a2,..,a6) is:

	a1	a2	a3	a4	a5	a6	Sum
a1		0	0	1	0	1	2
a2	0		0	1	0	1	2
a3	0	0		1	0	1	2
a4	0	0	0		0	0	0
a5	1	1	1	1		1	5
a6	0	0	0	1	0		1

This produces the following final rank (*Z*):

	1	2	3	4	5	6
Z:	a5	a1, a2, a3			a6	a4

The final ranking is presented to the decision-maker along with the credibility index which shows the outranking relation between every pair of alternatives. A sensitivity study can be conducted to investigate changes to the ranking order when the criteria weights, decision variables and thresholds are altered. Finally, a report can be generated or a file containing the decision information can be saved.

4.5.3 Implementation Overview

The flow diagrams in Figures 4-4, 4-5, 4-6 and 4-7 show that there are a range of controls and libraries needed to implement the ChemDecide framework. Some of these controls and libraries already exist in the .NET framework and external libraries but a number of these elements are required to be developed. Figure 4-9 shows the key algorithms and controls required for each of the four tools. A number of these are discussed in the subsequent sections.

a. Normalisation and Calculations

A function was developed to normalise values using the summation ratio normalisation method (equation 4-1) and the max scale normalisation procedure (equation 4-2). Similarly, mathematical calculations were developed as functions so that code is not repeated and the programming structure is straightforward and modular to follow.

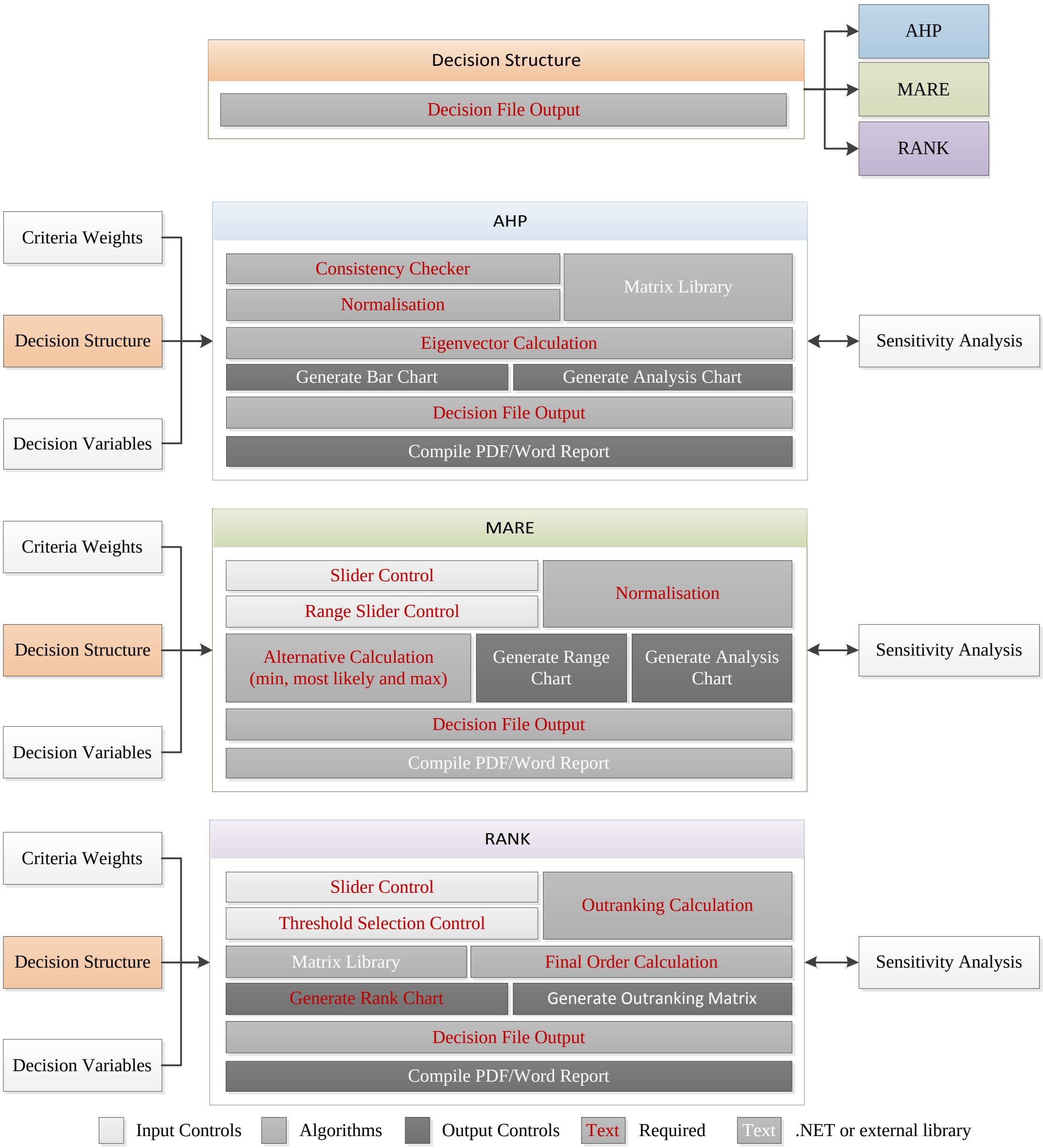


Figure 4-9 ChemDecide Implementation Overview

b. Slider, Range Slider and Threshold Selection Controls

The range slider control (Figure 4-1b) and the threshold selection control both require three moving bars. In the range slider, the three bars account for the minimum, most likely and maximum preference values whilst for threshold selection, the three bars represent the indifference, preference and veto thresholds. A slider bar control exists within the .NET Framework but it only allows for one moving bar. Therefore, a control needed to be built to handle the increased number of inputs. This was accomplished by forming rectangular boxes within a defined space and creating an event which is triggered when the user clicks the mouse button and the pointer is within the control. The event selects the nearest bar to the pointer and when the pointer is moved the bar follows the pointer until the mouse button has been released. Constraints were implemented to ensure that the bars cannot cross, meaning that the value of bar 1 is always less than bar 2 and the value of bar 2 is always less than bar 3.

c. Rank Chart

The RANK module produces three ranks, a descending rank, an ascending rank and a final rank. To display these, a control was developed that outputs the ranks as coloured textboxes. Often there are alternatives that receive a joint rank thus the control had to support multiple rows and columns of alternative boxes on three separate forms as illustrated in Figure 4-10.

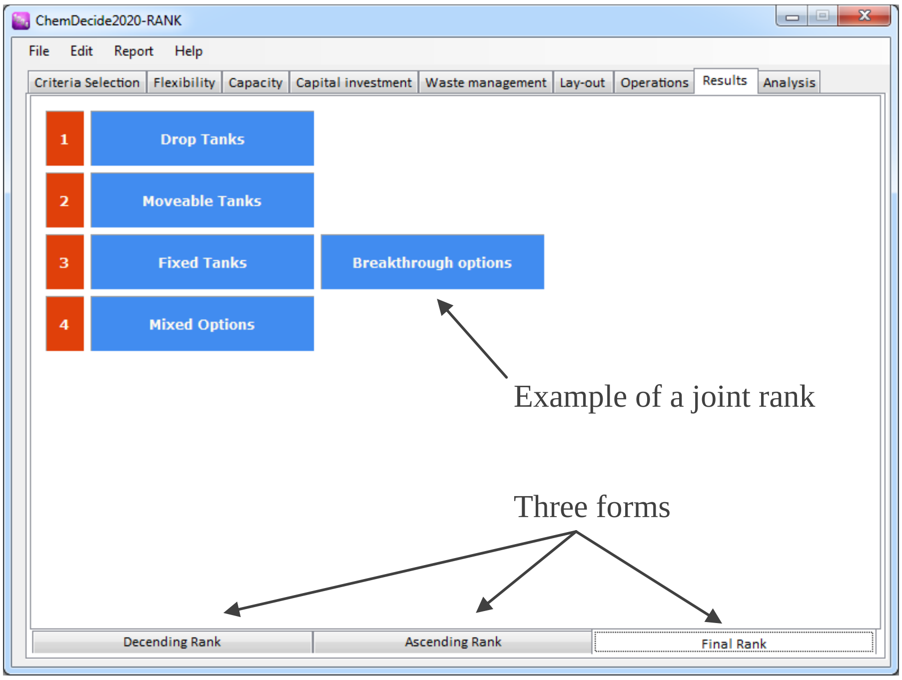


Figure 4-10 Example Chart in the RANK module

4.6 Conclusions

A methodology, Multi-Attribute Range Evaluations (MARE), was proposed for assisting in the decision-making process associated with the challenges arising in the implementation of Whole Process Design (WPD). The method, which is based on

Weighted Sum Method (WSM), allows a decision-maker to provide three values for each decision variable that captures the associated levels of uncertainty. To investigate the effectiveness of the MARE methodology, a framework has been developed that incorporates MARE and two other widely applied decision-making methods; Analytic Hierarchy Process (AHP) and ELECTRE III (RANK). The framework, ChemDecide, has been developed as a software package that can be distributed to industrial members for evaluation. The three methods are incorporated into the software as standalone tools that share similar interfaces and controls to ensure there is no bias between the methods. The aims are to compare the methods through the application of WPD decision-making case studies and to identify if the industrial requirements identified in Chapter 3 have been met through an industrial evaluation of the tools. The next chapter presents three WPD decision case studies along with a user evaluation of the ChemDecide framework.

"A good decision is based on knowledge and not on numbers"

Plato (380 B.C.)

5 Case Studies

5.1 Introduction

The previous chapter presented the Multi-Attribute Range Evaluations (MARE) methodology, the outcome of which allows a decision-maker to visually interpret their decision results with associated levels of uncertainty. To investigate the effectiveness of the MARE methodology, the ChemDecide framework was developed to incorporate MARE and two other widely applied decision-making methods; Analytic Hierarchy Process (AHP) and ELECTRE III (RANK). This chapter presents three industrial decision-making case studies that have been analysed using the three decision analysis modules in the ChemDecide framework. The underlying objectives of the case studies are to:

- Identify the effectiveness of each module for each decision-making case study by comparing the results, checking for inconsistences and assessing the decision-makers feedback.
- Validate the results of each analysis against the company's decision outcome.
- Identify which analysis method the decision-maker prefers in terms of input, output and in the handling of uncertainty.

These objectives will be considered in reaching a conclusion with regard to the overall aim of the case studies which is to identify which, if any of the tools, is most effective for decision-making in the implementation of Whole Process Design (WPD).

The first case study was provided by Robinson Brothers Ltd, the largest independent manufacturer of speciality organic chemicals in the United Kingdom. The goal of the study was to provide recommendations with regards to the selection of the best route to synthesise an undisclosed chemical. As identified from the analysis of the questionnaires (section 3.3.2), the route selection stage is one of the most common decision problems faced by managers when implementing WPD. The criteria weights and decision variables for this case study were generated during an interview with a business and technical development manager (section 3.2.1).

The second case study was the responsibility of a process engineering manager at GlaxoSmithKline (GSK). GSK is a pharmaceutical, biologics, vaccines and consumer healthcare company that operates globally. The goal of the study was to select an appropriate degasification technology for a new process. The final case study considered was overseen by a technology manager at Fujifilm Imaging Colorants Ltd, a global leader in innovative, high performance colorants for print and speciality applications. The objective of the study was to select the most appropriate combination of equipment to mix a substance in the early stages of process development. An interview transcript concerning the Robinson Brothers case study along with the data for all three case studies is included in Appendix C.

5.2 Route Selection (Robinson Brothers)

The objective of this case study was to provide recommendations with regard to selecting the best route to synthesise a chemical from three viable alternatives. The chemical name and chemistry is withheld for confidentiality reasons and hence the alternatives discussed below are referred to as routes one, two and three.

Five criteria (c1,c2,..,c5) were identified on which to base the decision (Table 5-1). The decision-maker could only quantify values for Product Yield (c1) in respect to each alternative. Therefore, the remaining four criteria were qualitative and measured by subjective preferences.

Table 5-1 Criteria for Robinson Brothers decision problem

		Source	Aim	Rationale
c1	Product Yield	Quantitative	Maximise	Maximising product yield maximises profit.
c2	Toxicity	Qualitative	Minimise	For safety and environmental concerns.
c3	Cost	Qualitative	Minimise	Minimising costs maximises profit.
c4	Ease of Separation	Qualitative	Minimise	Problems with separation could incur additional costs and time.
c5	Odour expulsion	Qualitative	Minimise	Robinson Brothers specialises in high odour containment but may still be a concern.

The underlying philosophy was to achieve the maximum amount of product at the lowest production cost. Ease of separation, levels of toxicity and odour expulsion were also included in the decision-making process as the decision-maker wished to minimise the complexity of the process and ensure compliance to external regulations. Route one provides substantial product yield at a low cost but issues could arise in terms of separation and excessive emissions of odour. Route two was much easier to develop but proved costly and provided the lowest amount of product yield. For route three, the product was easily separated, yield was reasonable and it was moderately expensive. However, it required highly toxic reagents for the synthesis.

5.3.1 AHP Analysis

The AHP module requires the input of pairwise comparisons to calculate criteria weights (section 2.2.4.2). The procedure for this is presented in section 4.5.2.2. Due to the nature of pairwise comparisons, requiring a selection for every possible pair of criteria rather than a single selection for each criterion, the analysis required ten pairwise comparisons to determine the criteria weights. The pairwise comparisons provided were valid in terms of transitivity (section 2.2.4.2) as the consistency checker indicated that the Consistency Ratio (CR) was below 0.8 (section 4.5.2.2). The criteria weights, which sum to 1, are shown as percentage values in Figure 5-1.

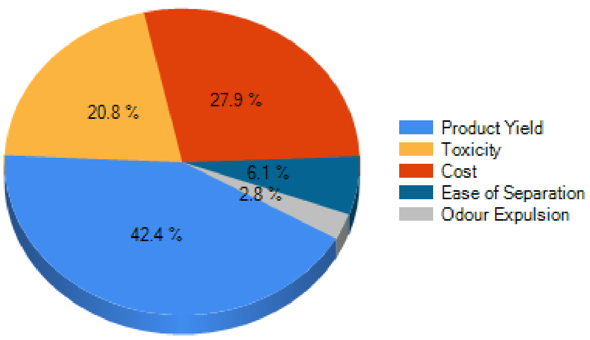


Figure 5-1 AHP criteria weights for the Robinson Brothers case study

From Figure 5-1, it can be concluded that c1 (‘product yield’) was prioritised, followed by c3 (‘cost’) and c2 (‘toxicity’). The remaining two criteria, c4 (‘ease of separation') and c5 ('odour expulsion') were deemed to be much less important in this analysis.

AHP also determines the decision variables in respect to the qualitative criteria by using pairwise comparisons. This was achieved by every possible pair of alternatives being compared four times, once for each of the four qualitative criteria. As there are three alternatives, only three pairwise comparisons are required with respect to each criterion. Similarly to the criteria weights, the pairwise selections were determined as valid in terms of transitivity as each consistency check indicated that the CR was below 0.8. To determine the decision variables with respect to the one quantitative criterion, a value is required for each alternative. Thus, for c1 ('product yield'), three estimated percentage values were given, one for each of the three alternatives.

The software tool calculated the results (section 4.5.2.2) and presented them in a chart (Figure 5-2) along with a graphical representation of the decision variables (Figure 5-3).

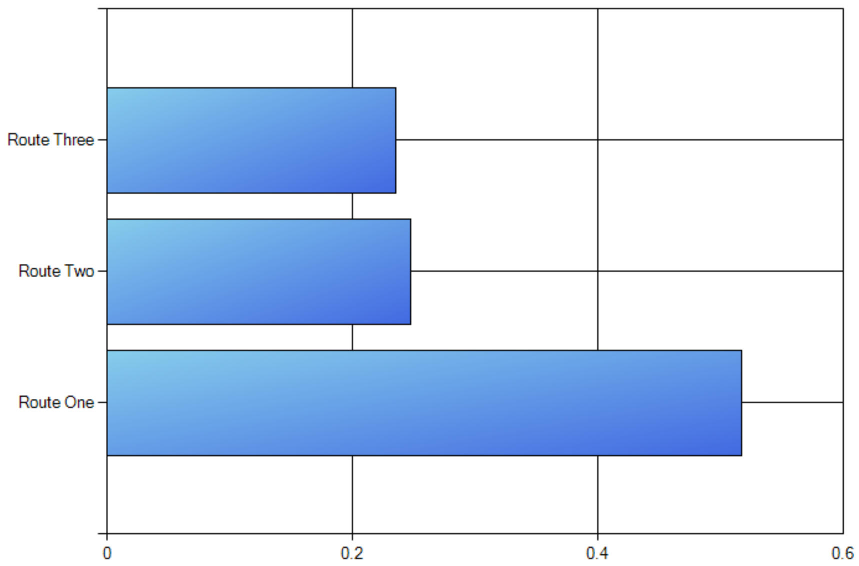


Figure 5-2 Final scores of the AHP analysis for the Robinson Brothers case study

Figure 5-2 shows that route one achieved the highest overall score and it was double that of the other two possible routes. This was due to c1 ('product yield'), c2 ('toxicity') and c3 ('purchase price') being the most influential criteria and as shown in Figure 5-3, route one scored the highest in all three categories. Route two performed well in terms of c2 ('toxicity'), c4 ('ease of separation') and c5 ('odour expulsion') while route three performed well in terms of c1 ('product yield') and c4 ('ease of separation'). Both routes achieved similar scores as the criteria weightings balanced the impact of the decision variables.

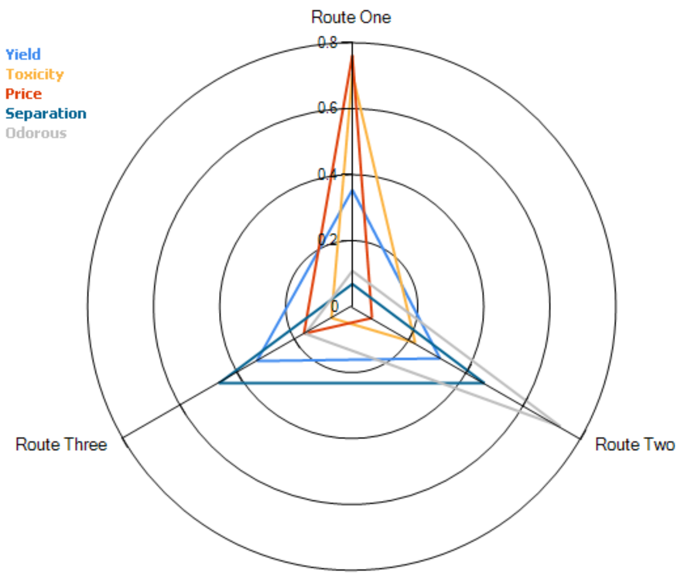


Figure 5-3 AHP decision variables for the Robinson Brothers case study

5.3.2 MARE Analysis

Unlike AHP, the MARE and RANK modules require a selection for each criterion to determine the criteria weights. Therefore, in the MARE and RANK analyses, five selections were required to determine the criteria weights. These values are normalised to sum to 1 as shown in section 4.3. As the values for this case study were generated from an interview (Appendix C), the criteria weights for the MARE and RANK analyses were adjusted to correspond with the AHP analysis. This ensured the values remained consistent throughout the three analyses. The MARE and RANK criteria weights are shown in Figure 5-4 as percentage values.

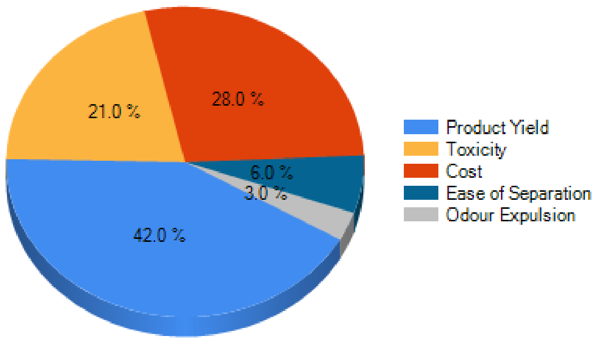


Figure 5-4 MARE and RANK criteria weights for the Robinson Brothers case study

In terms of decision variables, the MARE module requires one selection (most likely value) if the decision-maker is certain and three selections (minimum, most likely and maximum) if the decision-maker is uncertain about a particular selection. To keep the decision variables consistent to the AHP analysis, the likely values for the MARE analysis were based on the eigenvector outputs from the AHP analysis. Uncertainty ranges (minimum and maximum values) were applied to all of the decision variables with the maximum set at 2% more than the likely values and the minimum being set at 2% less. The MARE tool calculated the results, as shown in section 4.3, and output a results chart (Figure 5-5) along with a graphical representation of the most likely decision variables (Figure 5-6).

Figure 5-5 shows that route one was the best alternative as the entire range (minimum to maximum) had higher preference scores than the most likely values of routes two and three. This is a consequence of route one performing well in terms of c1 ('product yield'), c2 ('toxicity') and c3 ('purchase price') which are the most influential criteria as shown in Figure 5-4. The most likely value of route two scored marginally better than route three. Figure 5-6 shows this is because route two performed better in terms of c2 ('toxicity'), c4 ('ease of separation') and c5 ('odour expulsion') while route three only outperformed route two in terms of c1 ('product yield') and c4 ('ease of separation').

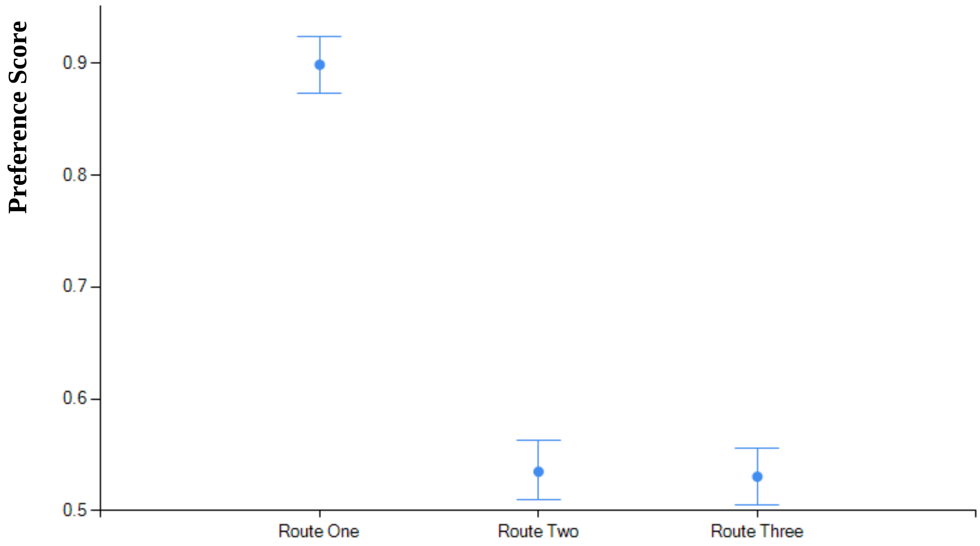


Figure 5-5 Final scores of the MARE analysis for the Robinson Brothers case study

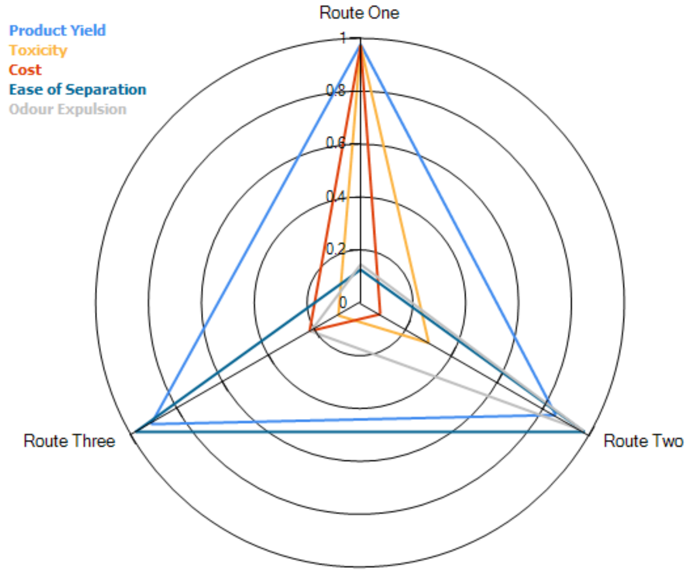


Figure 5-6 MARE likely decision variables for the Robinson Brothers case study

5.3.3 RANK Analysis

As explained in the previous section, the RANK analysis utilised the same criteria weights as the MARE analysis, thus the RANK criteria weights are shown in Figure 5-4. In terms of decision variables, the RANK module required the input of a single score for each alternative with respect to each criterion. For consistency, these values were chosen to directly correspond to the most likely values in the MARE analysis. The only dissimilarity between the RANK and MARE analyses was that three threshold values (indifference, preference and veto) were required for each criterion (section 4.5.2.4). These values were selected depending upon the variation of the decision variables. The RANK tool calculated the results as shown in section 4.5.2.4 and three rank orders were output, one for the descending distillation, one for the ascending distillation and another one for the final rank (Figure 5-7). Additionally, the credibility matrix was displayed to show the outranking relationship for every pair of alternatives (Figure 5-8).

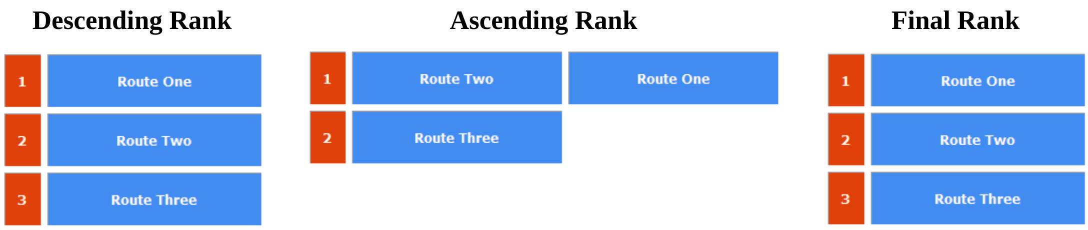


Figure 5-7 Results of the RANK analysis for the Robinson Brothers case study

	Route One	Route Two	Route Three
Route One	N/A	0.000	0.940
Route Two	0.000	N/A	0.440
Route Three	0.000	0.000	N/A

Ranked Better Incomparable Indifferent Ranked Worse

Figure 5-8 RANK Credibility index for the Robinson Brothers case study

Similar to the AHP and MARE analyses, Figure 5-7 shows that route one outperformed routes two and three for the descending and final rank. However, in the ascending distillation, route one and route two jointly achieved first rank. Figure 5-8 shows that this occurred due to routes one and two attaining an identical outranking relationship (0.000).

5.3.4 Evaluation

All three analyses were provided with similar data with the only variations being the threshold values in RANK, the uncertainty ranges in MARE and the slight differences in the decision variables in AHP due to the eigenvector calculations. The results from all three analyses were identical on an ordinal scale (Route 1 > Route 2 > Route 3). However, the RANK tool positioned route two as a close second to route one while AHP and MARE gave route two and three similar scores, far below what route one attained.

From conducting a sensitivity analysis on the RANK tool, it was identified that this situation occurred due to the veto thresholds (a threshold at which the decision-maker ultimately prefers one alternative over another and wishes to select that alternative with total certainty). If all of the veto thresholds were set to their maximum (100) which effectively removes them from the analysis (Sayyadi & Makui, 2012), the outranking relationship between route one and route two significantly changes, positioning route two as a much less attractive alternative. This can be seen in the credibility index in Figure 5-9 where route one outranks route two by 0.910 and route two outranks route one by 0.025. However, this change impacted on the order of results in the RANK analysis, effectively placing route three as a more attractive alternative to route two as shown in Figure 5-10.

	Route One	Route Two	Route Three
Route One	N/A	0.910	0.940
Route Two	0.025	N/A	0.440
Route Three	0.024	0.830	N/A

Ranked Better | Incomparable | Indifferent | Ranked Worse

Figure 5-9 RANK Credibility index after removing the veto thresholds

Figure 5-9 shows that this is a consequence of route three outranking route two by 0.830 and route two outranking route three by only 0.440.

Figure 5-10 Result of RANK after removing the veto thresholds

5.3.5 Conclusions

The aim of this case study was to recommend the best route to synthesise a chemical from three viable alternative routes. There were no inconsistencies between the three methods as the criteria weights and decision variables were adjusted to correspond to the AHP analysis. In general, all approaches recommended the same results. This supported the claims of Huang et al. (2011) who stated "*an important observation ... is that all* [MCDA methods] *tend to favour the same alternatives*". However, it was identified that the results of the RANK analysis were strongly dependent on the given thresholds. When using veto thresholds, route two performed similarly to route one. With the veto thresholds removed, route two performed similarly to route three which is more comparable to the AHP and MARE analyses.

Robinson Brothers, who also evaluated the decision using their techniques (described in section 3.2.1), revealed the following: *"With all things considered we evaluated only route one and the separation of the required product from the by-products (mostly inorganic) proved insurmountable and the project was discontinued"*. This outcome validates the recommendations provided by the three analysis methods.

5.3 Degassing Methodology Selection (GSK)

The goal of this case study was to select an appropriate degasification technology for a new chemical development process. The study was the responsibility of a process engineering manager for GlaxoSmithKline (GSK). Along with the decision-maker, one other person was present during the analysis. Details of the product and process are withheld for reasons of confidentiality. The decision-makers initially identified five alternatives (Table 5-2) and five criteria (Table 5-3) on which to base the decision.

Table 5-2 Alternatives for GSK case study

a1	Packed Column
a2	Membrane
a3	Duty Standby CSTR - Vacuum
a4	Duty Standby CSTR with Sparge
a5	Ultrasonic

Table 5-3 Criteria for GSK case study

		Source	**Aim**	**Rationale** (from the decision-makers)
c1	Minimises Hold Up	Qualitative	Minimise	*"Supports the economics of the process and ease of operation."*
c2	Simple to Build	Qualitative	Minimise	*"Simplicity in build will speed up development. Must increase robustness of the solution and make the equipment easier to clean. This will contribute to a lower cost."*
c3	Technically Possible	Quantitative	Maximise	*"The solution has to be capable of removing the gas from the solution to a low enough level."*
c4	Available Now	Qualitative	Maximise	*"Need to test and place orders now, solutions not off the shelf need to be excluded."*
c5	Low Cost	Qualitative	Minimise	*"Lower the cost, the better the project payback."*

As shown in Table 5-3, the underlying philosophy for the company was to select a technology that was inexpensive, available and straightforward to implement. From the five alternatives in Table 5-2, only four were technically viable. Ultrasonic (a5) was not capable of removing enough gas from the solution but was included in the analyses as it could be a viable alternative in the future if advances are made in the technology. The least expensive alternatives were Packed Column (a1) and Membrane (a2). However, these options were not readily available to implement quickly within GSK. The best options in terms of availability were the two Duty Standby CSTR alternatives (a3 and a4).

5.3.1 AHP Analysis

As there are five criteria, the AHP module required ten pairwise comparisons to determine the criteria weights (section 2.2.4.2). These are shown as percentage values in Figure 5-11. The consistency check (section 4.5.2.2) determined that the CR was below 0.8, indicating that the pairwise comparisons were transitive and therefore consistent.

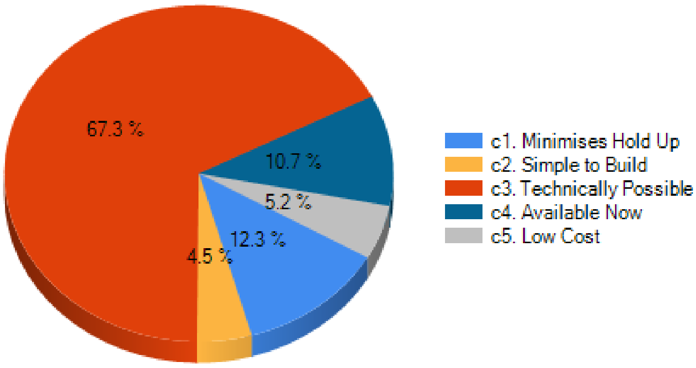


Figure 5-11 AHP criteria weights for the GSK case study

Figure 5-11 shows that the only quantitative criterion, c3 ('technically possible'), achieved the most influential weight accounting for over two thirds of the entire criteria weighting. The decision-makers chose to use binary logic to define the alternative values with respect to this criterion. The binary logic associated 1 with a positive, i.e. technically feasible and 0 as unfeasible. As Ultrasonic (a5) was the only technically unfeasible alternative, this criteria weighting scheme prevented this option from scoring highly.

As there are five alternatives, ten pairwise comparisons were required to define the decision variables for each the four qualitative criteria. In addition, a numerical value was required for each of the five alternatives with respect to the one quantitative criterion. Each of the pairwise comparison sets in respect to the decision variables had a CR below 0.8 indicating that they were transitive / consistent. The AHP module calculated the results (section 4.5.2.2) and presented them in a chart (Figure 5-12) along with a graphical representation of the decision variables (Figure 5-13).

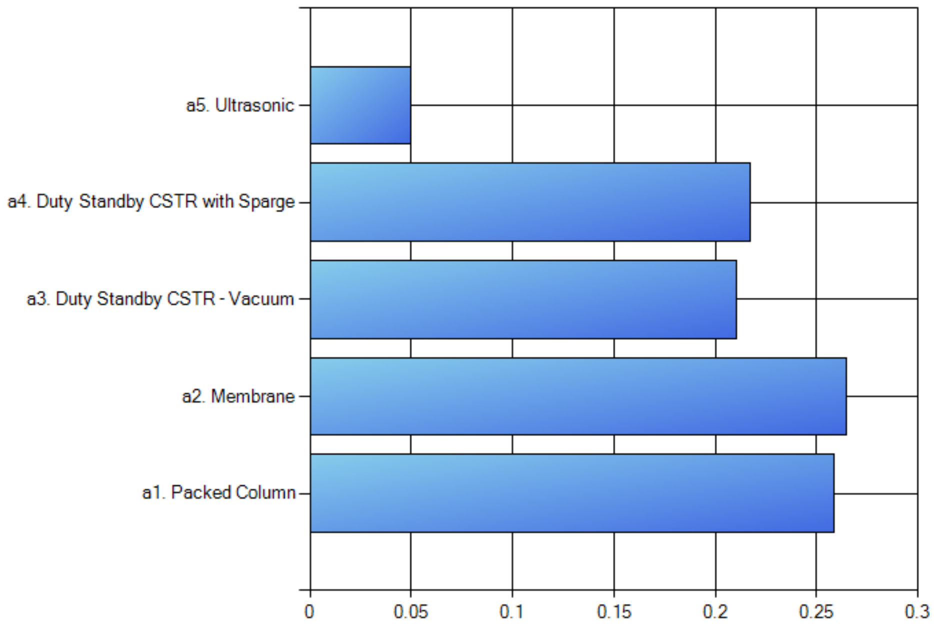


Figure 5-12 Final scores of the AHP analysis for the GSK case study

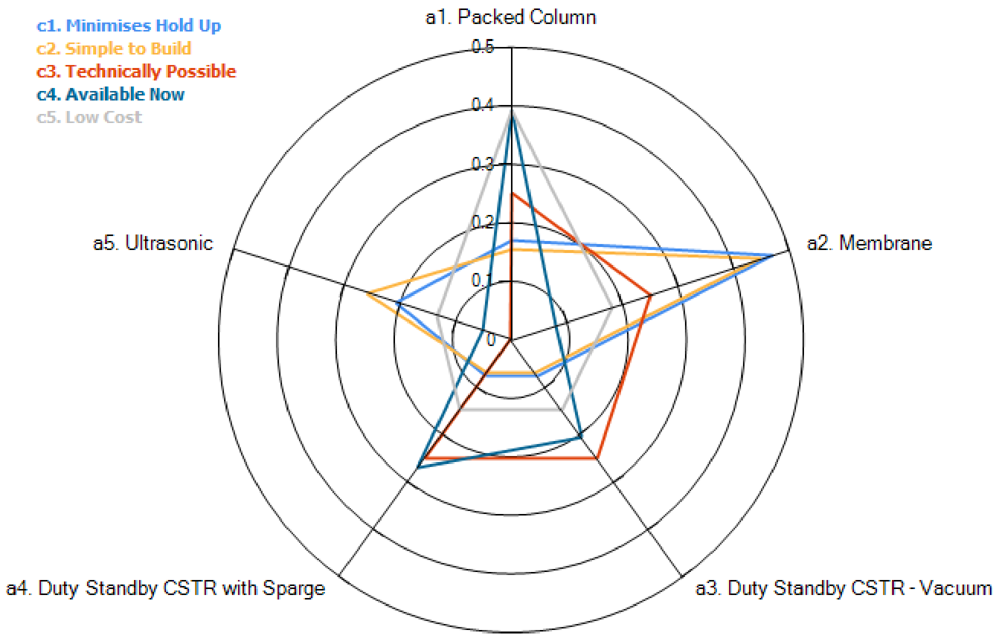


Figure 5-13 AHP decision variables for the GSK case study

Figure 5-13 shows that Membrane (a2), which was the highest scoring alternative (Figure 5-12), performed well in terms of c1 (‘minimises hold up’) and c2 (‘simple to build’). The second best alternative Packed Column (a1) performed well in terms of c4 (‘available now’) and c5 (‘low cost’).

The alternatives related to Duty Standby CSTR (a3 and a4) achieved similar but lower scores than the two best alternatives (Figure 5-12). Ultrasonic (a5), attained the lowest score as it was the only alternative to be set as infeasible (0) in terms of c3 (‘technically possible’), the most influential criterion with respect to weight.

5.3.2 MARE Analysis

The MARE module required five slider bar selections from the decision-makers to determine the criteria weights (Figure 5-14). Similar to the AHP analysis, the most influential criterion was c3 (‘technically possible’). However, this criterion attained a much lower weight of less than a third in comparison to over two thirds in the AHP analysis. This meant that the other four criteria attained higher weights, resulting in them having more impact on the analysis.

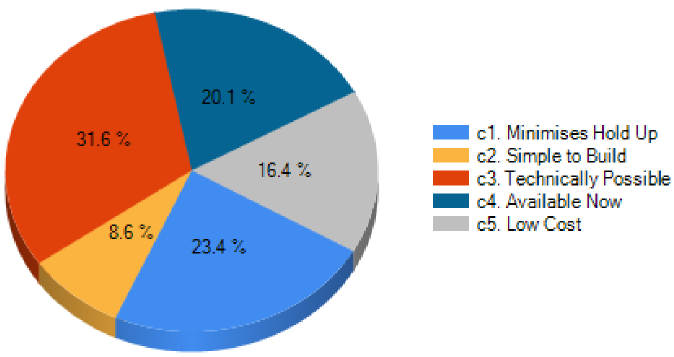


Figure 5-14 MARE criteria weights for the GSK case study

The decision-makers used the same binary logic as for the AHP analysis to define the decision variables for c3 (‘technically possible’). Consequently, minimum and maximum values were not utilised. However, minimum and maximum selections were given for all of the alternatives with respect to the qualitative criteria.

The MARE module calculated the results (section 4.3) and output a results chart (Figure 5-15) along with a graphical representation of the most likely decision variables (Figure 5-16).

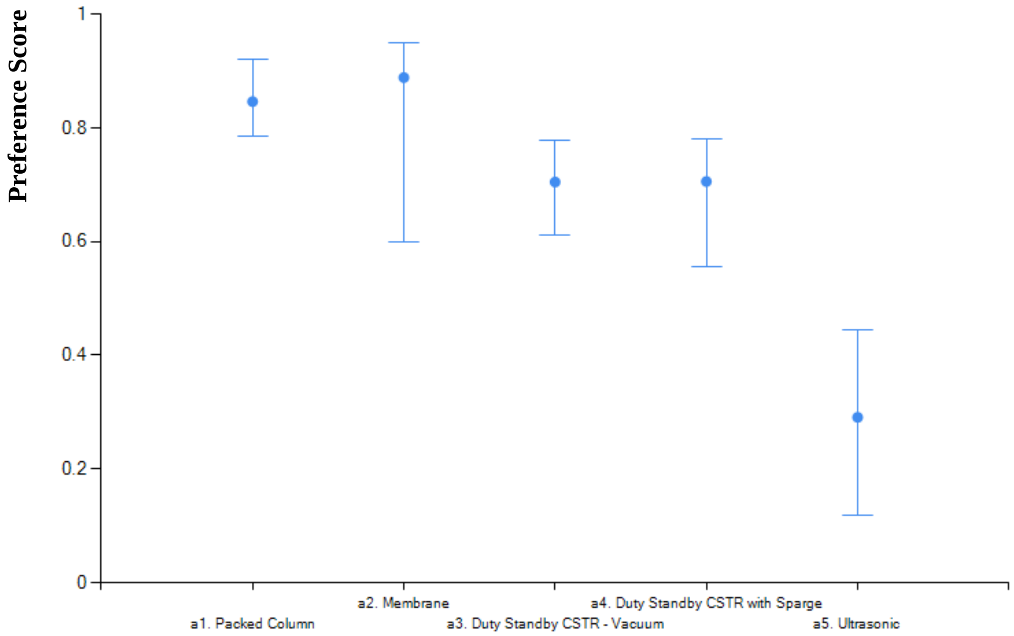


Figure 5-15 Final scores of the MARE analysis for the GSK case study

Figure 5-15 shows that Membrane (a2) scored marginally better than Packed Column (a1) in terms of the most likely score but it has a larger uncertainty range. Consequently, Packed Column (a1) may be a more attractive alternative as it is more certain to perform within a higher range. Membrane (a2) could, in a worst case scenario, be inferior to Packed Column (a1) and the alternatives related to Duty Standby CSTR (a3 and a4). The uncertainty associated with the Membrane (a2) option cannot be seen in the AHP analysis, thus the AHP result could be very misleading.

The most likely decision variables (Figure 5-16) show that Membrane (a2) scored higher than Packed Column (a1) due to performing well in terms of c1 (‘minimise hold up’) and c2 (‘simple to build’). Nevertheless, Packed Column (a1) outperformed Membrane (a2) in terms of c4 (‘available now’) and scored highly in terms of c5 (‘low cost’). Ultrasonic (a5), similarly to the AHP analysis, achieved the lowest overall score. The two Duty Standby CSTR options (a3 and a4) achieved similar results with Duty Standby CSTR with Sparge (a4) only marginally outperforming Duty Standby CSTR - Vacuum (a3) in terms of most likely value. Considering the uncertainty in Duty Standby CSTR with Sparge (a4) is higher than Duty Standby CSTR - Vacuum (a3), the latter option may be a better choice. However, in the results of AHP (Figure 5-12) the difference between the two alternatives is much larger, indicating that Duty Standby CSTR with Sparge (a4) is a better choice.

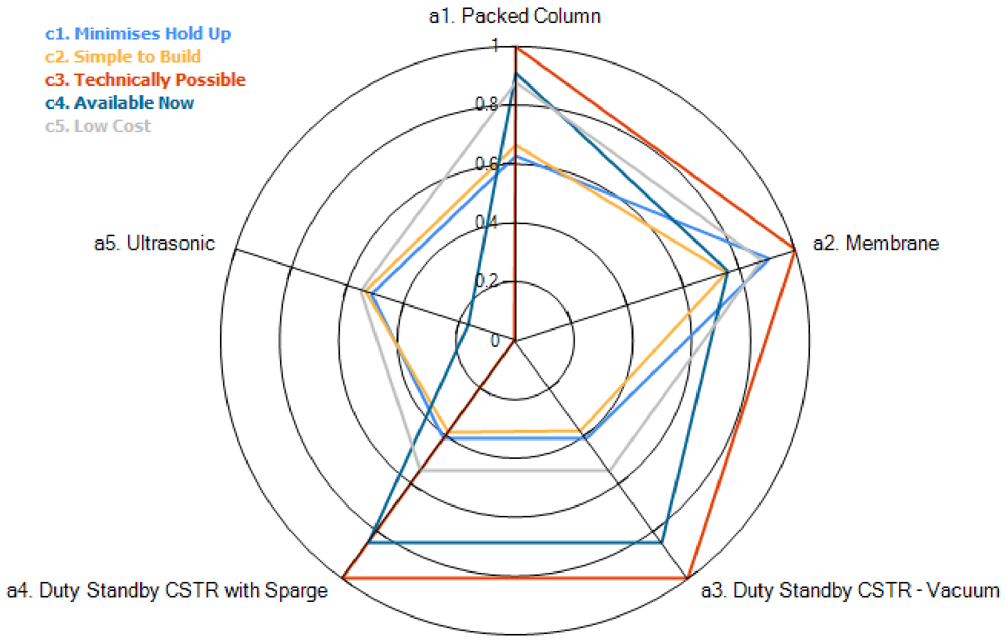


Figure 5-16 MARE most likely decision variables for the GSK case study

5.3.3 RANK Analysis

As for the MARE module, the RANK module required five slider bar selections from the decision-makers to determine the criteria weights (Figure 5-17). Similarly, the most influential criterion was c3 ('technically possible') followed by c1 ('minimise hold up') and c4 ('available now'). However, the percentage weights in RANK where different to MARE, with c2 ('simple to build') scoring higher and c5 ('low cost') scoring lower than the MARE analysis. This will be discussed in section 5.3.4.

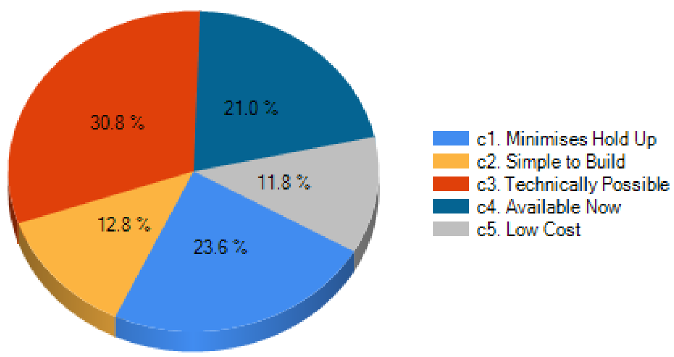


Figure 5-17 RANK criteria weights for the GSK case study

The decision-makers used the same binary logic to determine the decision variables with respect to c3 ('technically possible') and provided slider bar selections for each alternative in respect to each qualitative criterion. They also provided indifference, preference and veto thresholds for each criterion.

The RANK tool calculated the results and displayed three rankings as shown in Figure 5-18. Additionally, the credibility matrix was displayed which shows the outranking relationship for every pair of alternatives (Figure 5-19).

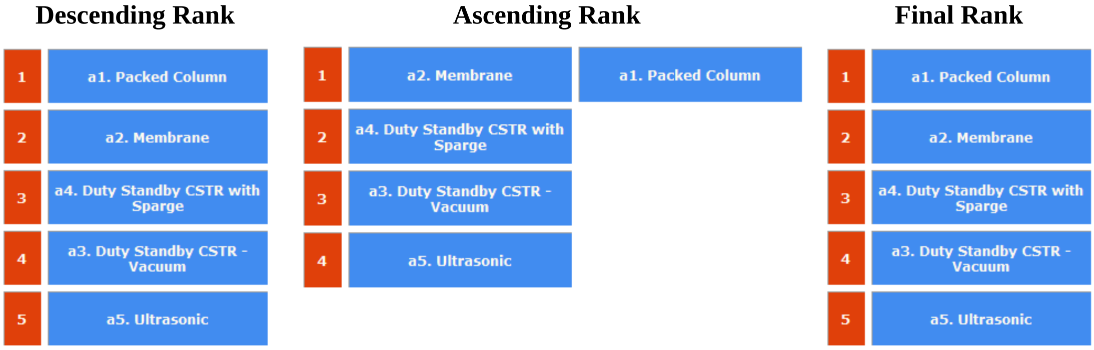


Figure 5-18 RANK Results Chart for the GSK decision problem

The ascending distillation placed Membrane (a2) and Packed Column (a1) as joint best alternatives while the descending distillation placed Packed Column (a1) as the single best alternative. As a consequence, the final order classification (discussed in section 4.5.2.4), placed Packed Column (a1) as the best alternative in the final rank. The rank order of the remaining three alternatives (a4, a3 and a5) was identical to that of the AHP and MARE analyses.

	a1. Packed Column	a2. Membrane	a3. Duty Standby CSTR - Vacuum	a4. Duty Standby CSTR with Sparge	a5. Ultrasonic
a1. Packed Column	N/A	0.780	1.000	1.000	0.858
a2. Membrane	0.696	N/A	0.804	0.804	1.000
a3. Duty Standby CSTR - Vacuum	0.420	0.636	N/A	0.827	0.713
a4. Duty Standby CSTR with Sparge	0.577	0.636	1.000	N/A	0.704
a5. Ultrasonic	0.049	0.422	0.279	0.279	N/A

Ranked Better Incomparable Indifferent Ranked Worse

Figure 5-19 RANK Credibility index for the GSK case study

The credibility matrix (Figure 5-19) shows that Packed Column (a1) outranked Membrane (a2) by 0.780 while Membrane (a2) outranked Packed Column (a1) by

0.696 resulting in Packed Column (a1) achieving a better rank in the descending distillation and subsequently, the final rank.

5.3.4 Evaluation

By comparing the criteria weights (Figure 5-20) and decision variables (Figure 5-21) for the three analyses, it is evident that there are a number of inconsistencies. The most noticeable discrepancy was the weighting that AHP placed on the decision-makers' weights and scores. Figure 5-20 shows that c3 ('technically possible') was the most important criterion for all three analyses but that AHP weighted this criterion much more highly than MARE and RANK. As a result, the remaining four criteria in the AHP analysis received much lower weights than MARE and RANK.

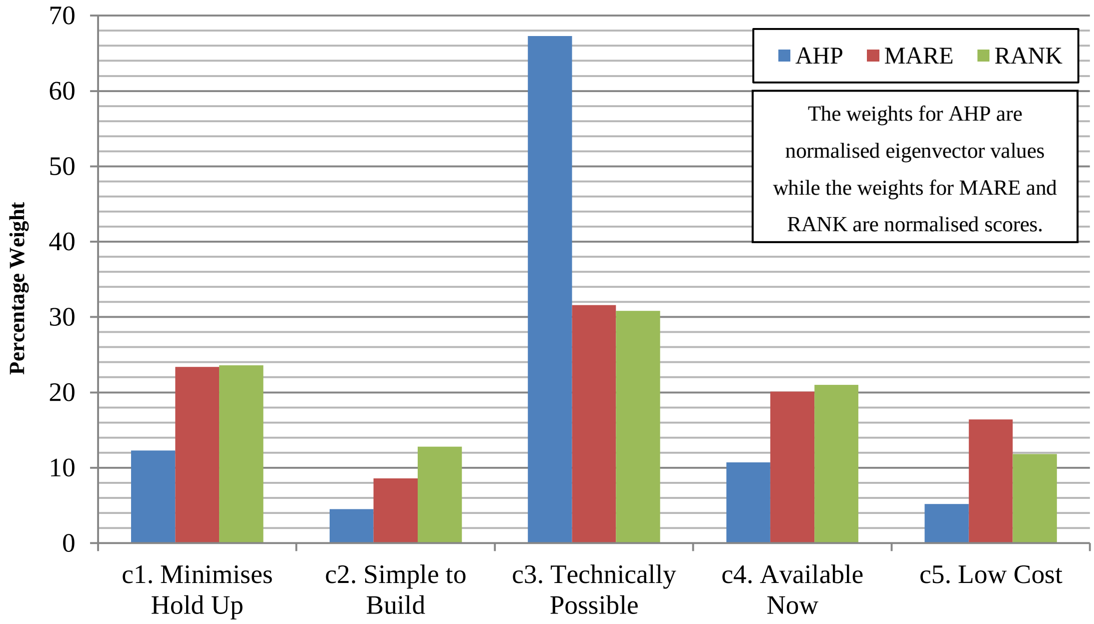


Figure 5-20 Comparison of the criteria weights for the GSK case study

From studying Figure 5-21, it is clear that AHP has also exaggerated the decision-maker's preferences with regard to the decision variables. The decision variables for the four qualitative criteria (c1, c2, c4, c5) show that AHP has increased scores for the better alternatives (a2 in respect to c1, a2/a5 in respect to c2, a1 in respect to c4 and a1 in respect to c5) and decreased scores for the inferior alternatives (a3/a4 in respect to c1/c2, a2 in respect to c4 and a4/a5 in respect to c5) in relation to the MARE and RANK analyses.

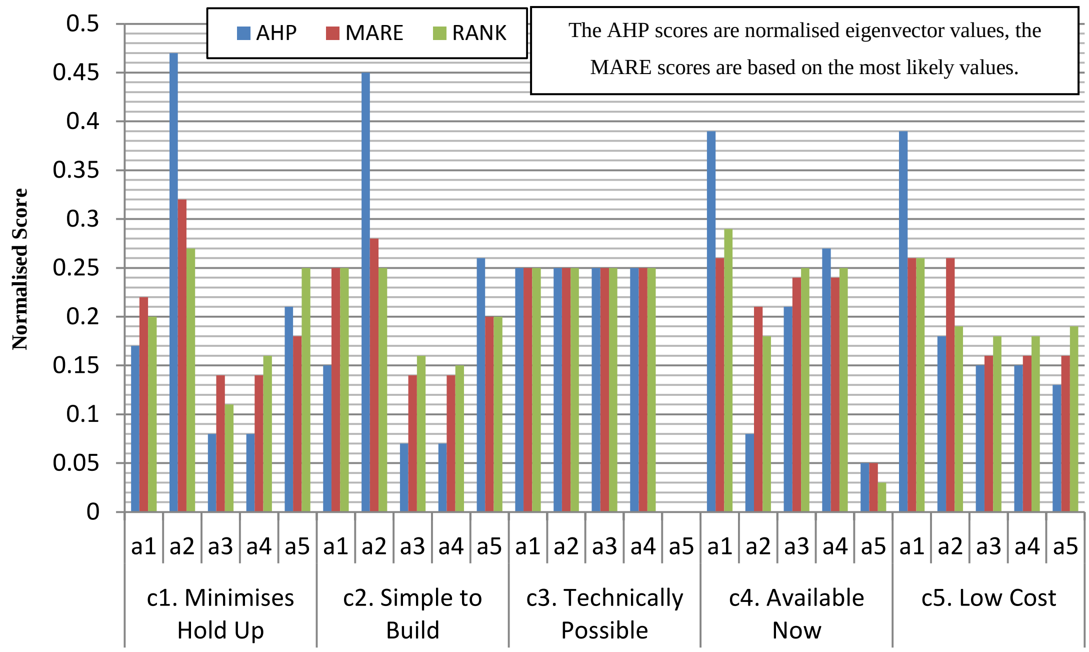


Figure 5-21 Comparison of the decision variables for the GSK case study

As MARE and RANK share identical inputs for expressing criteria weights and decision variables in relation to the qualitative criteria (slider bars), their criteria weights and decision variables should be similar. However, Figure 5-20 and Figure 5-21 show a number of inconsistencies within these selections.

The criteria weights, c2 ('simple to build') and c5 ('low cost') showed the greatest dissimilarities whilst for the decision variables, a2 and a5 for c1 ('minimises hold up') and a2 for c5 ('low cost') showed the greatest variation. The causes of these inconsistencies will be investigated and discussed in the subsequent chapter.

However, two questions arise from these inconsistencies:

- Have the three analyses recommend the same results despite the inconsistencies?
- Which weighting scheme correctly represents the decision-makers' preferences?

Considering question one, the RANK tool provides results in the form of an ordinal ranking, thus the outputs of the three analyses were not comparable on a numerical scale. Therefore, the results of the analyses were evaluated by means of an ordinal scale. Table 5-4 shows that the three analyses attained similar results except for the RANK analysis which recommended a1 ahead of a2.

Table 5-4 Comparison of the three analyses results in the form of an ordinal rank

	1st	2nd	3rd	4th	5th
AHP	a2	a1	a4	a3	a5
MARE (Most Likely value)	a2	a1	a4	a3	a5
RANK	a1	a2	a4	a3	a5

Although the MARE and AHP analyses had significantly different criteria weights, their results in the form of an ordinal ranking were identical. This would indicate that the results are not strongly dependent on the criteria weights. To test this hypothesis, a sensitivity study was performed on the RANK criteria weights to see if the application of the AHP, MARE or the average weights of all three analyses would change the order of the results to match the AHP and MARE analyses. As shown in Table 5-5, the MARE and average weighting schemes did not affect the order. However, the application of the AHP weights resulted in a1 and a2 becoming joint best alternatives and a3 and a4 becoming joint second best alternatives.

Table 5-5 Sensitivity study of the RANK criteria weights

RANK using:	1st	2nd	3rd	4th	5th
AHP weights	a1, a2		a3, a4		a5
MARE weights	a1	a2	a4	a3	a5
Average weights	a1	a2	a4	a3	a5

To assess if the variations in the decision variables affected the result of the RANK analyses, the most likely decision variables for MARE were applied to the RANK decision variables and the RANK decision variables were applied to the most likely decision variables in the MARE analysis. The criteria weights and threshold values (in RANK) remained constant. Table 5-6 shows that by applying the decision variables of MARE to the RANK analysis, the best alternative changes from a1 to a2, placing a1 as the second best alternative. Similarly, by applying the decision variables of RANK to the MARE analysis, the best alternative changes from a2 to a1, placing a2 as second best. Therefore, the inconsistencies in the decision variables are responsible for a1 being preferred over a2 in the RANK results.

Table 5-6 Sensitivity study of the RANK and MARE decision variables

	1st	2nd	3rd	4th	5th
RANK *(using MARE most likely values as the decision variables)*	a2	a1	a3, a4		a5
MARE *(using RANK decision variables as the most likely values)*	a1	a2	a4	a3	a5

5.3.5 Post Analyses Interview

After conducting the three analyses, the decision-maker made time to review his experiences and to discuss the results. Overall, the decision-maker's preferred tool was MARE as it allowed the user to "*spread their answers*" and "*it was much more useful in terms of seeing the uncertainty behind the membrane option*". He explained that Membrane (a2) would have been the favoured alternative internally within the company if it had been possible to reduce the uncertainty associated with it. However, post analysis, he favoured Packed Column (a1), as that alternative was more certain to perform well (section 5.3.2). This option was selected as the best alternative based on the team's intuition prior to the analysis.

In terms of data entry, the decision-maker preferred MARE and RANK as the AHP consistency check was "*somewhat disconcerting*" and he stated that straight data entry was faster in contrast to pairwise comparisons. Nevertheless, when asked about the differences in the criteria weights, the decision-maker said the weights produced by AHP were more representative. His reasoning was that c3 ('technically possible') was a "*veto type attribute*" and AHP weighted this criterion much higher.

Considering the analysis output, the decision-maker preferred MARE to AHP and AHP to RANK. He explained that the RANK credibility index (Figure 5-19) was "*confusing*" and that he disliked output in the form of an ordinal ranking as the differences between the alternatives were not clear.

When considering the framework as a whole, the decision-maker liked how the three analyses tools forced a structured discussion about a decision problem and how they produced documentation for future reference. He said overall that the tools were easy to use and that the framework "*with a bit of discipline, might be a standard tool we could use*".

5.3.6 Conclusions

The aim of this particular case study was to identify an appropriate degasification methodology for a new chemical development process. The AHP and MARE analyses recommended the same results on an ordinal scale. The RANK analysis delivered a slightly different ordering, placing Packed Column (a1) ahead of Membrane (a2). It was identified that the contrasting result was a result of the inconsistencies in the qualitative decision variables provided by the decision-maker. These inconsistencies are investigated and discussed further in Chapter 6.

Post analyses, the decision-maker selected Packed Column (a1) as this option performed well in all three analyses and there was less uncertainty associated with it in comparison to Membrane (a2). The larger uncertainty linked to the Membrane (a2) option compared with Packed Column (a1) was only identified by the MARE analysis. In summary, the MARE module was favoured for this particular decision problem.

5.4 Premix Equipment Selection (FFIC)

The decision analysis was the responsibility of a technology manager at Fujifilm Imaging Colorants Ltd (FFIC). Along with the technology manager, eight other people were present during the analysis. The decision was to select the optimum equipment to mix a substance in the early stages of process development (a process which the decision-maker refers to as premixing). The product and different equipment options were not disclosed for confidentiality reasons hence the four alternatives are referred to as method 1, 2, 3 and 4. The decision-maker and team identified ten criteria on which to base their decision (Table 5-7).

The requirement was to select an equipment option which is inexpensive, straightforward and reliable to operate. Of the ten criteria chosen to model the decision, two were quantitative and represented by estimated values of capital expenditure for producing different capacities of product. Criterion c1 (‘capital cost at 50’) referred to the initial design capacity and c2 (‘capital cost at 100’) is the capacity if future expansion is required. The eight qualitative criteria were related to the ease and reliability of production and thus, as no quantitative data was available, they were represented by the decision-makers’ subjective preferences.

Table 5-7 Criteria for FFIC premix equipment selection problem

		Source	Aim	Rationale (from the decision-maker)
c1	Capital cost at 50	Quantitative	Minimise	*"Capital expenditure is limited."*
c2	Capital cost at 100	Quantitative	Minimise	
c3	Ease of clean down	Qualitative	Maximise	*"Multi-product plant."*
c4	Complexity of solids feeding required	Qualitative	Minimise	*"Different options may place different demands on solids feeding equipment."*
c5	Ease of operation	Qualitative	Maximise	*"Multiple concurrent operations on plant."*
c6	Mechanical reliability	Qualitative	Maximise	*"Impact of outage significant."*
c7	Material losses	Qualitative	Minimise	*"Material is of high value."*
c8	Ease of modelling at laboratory scale	Qualitative	Maximise	*"Lab tests may be required."*
c9	Quality of vendor support	Qualitative	Maximise	*"Rapid support is necessary."*
c10	Power requirements	Qualitative	Minimise	*"Power needs kept to a minimum."*

Of the four equipment options, method 4 was the least expensive in terms of running costs. However, this equipment option was difficult to clean, had poor vendor support, would lose considerable amounts of valuable material during operation and was challenging to model at a laboratory scale. Methods 1 and 2 would have the lowest running costs at the current rate of production but would become more expensive if expansion was required. The running costs of implementing method 3 would remain constant if expansion was required but this method would lose the highest amount of valuable material, had the highest power consumption and would be difficult to clean.

5.4.1 AHP Analysis

Due to the large number of criteria in this analysis, AHP required 35 pairwise comparisons to calculate the criteria weights. Although this necessitated significant levels of input, the resulting pairwise comparisons were consistent (with a CR below 0.8) and the weights as percentage values are shown in Figure 5-22.

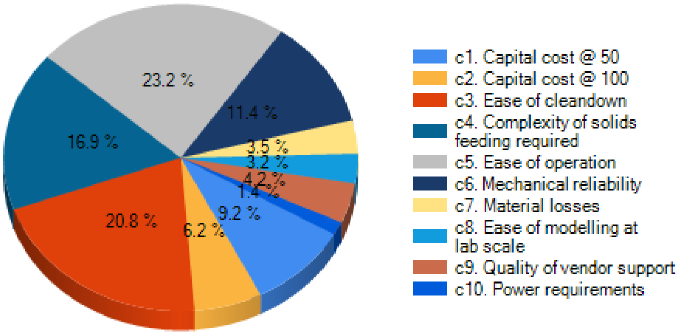


Figure 5-22 AHP criteria weights for the FFIC case study

Figure 5-22 shows that the most influential criteria in order of importance were c5 ('ease of separation'), c3 ('ease of cleandown'), c4 ('complexity of solids feeding required') and c6 ('mechanical reliability').

With four alternatives, the decision-maker was required to select six pairwise comparisons for each qualitative criterion and enter four numerical values for each quantitative criterion. The consistency checks determined that each pairwise comparison set had a CR below 0.8 indicating that the selections were transitive and consistent.

The AHP module calculated the results (Figure 5-23) and presented a graphical representation of the decision variables (Figure 5-24). Figure 5-24 shows that method 4, which was the highest scoring alternative (Figure 5-23), performed well in terms of c1 ('capital cost at 50'), c4 ('complexity of solids feeding required') and c6 ('mechanical reliability'). Methods 1 and 3 attained similar scores (Figure 5-23), with method 1 performing well in terms of c3 ('ease of cleandown'), c8 ('ease of modelling at lab scale') and c10 ('power requirements') and method 3 performing well in terms of c4 ('complexity of solids feeding required') and c5 ('ease of operation'). Method 2 achieved the lowest overall score but performed well in terms of c7 ('material losses').

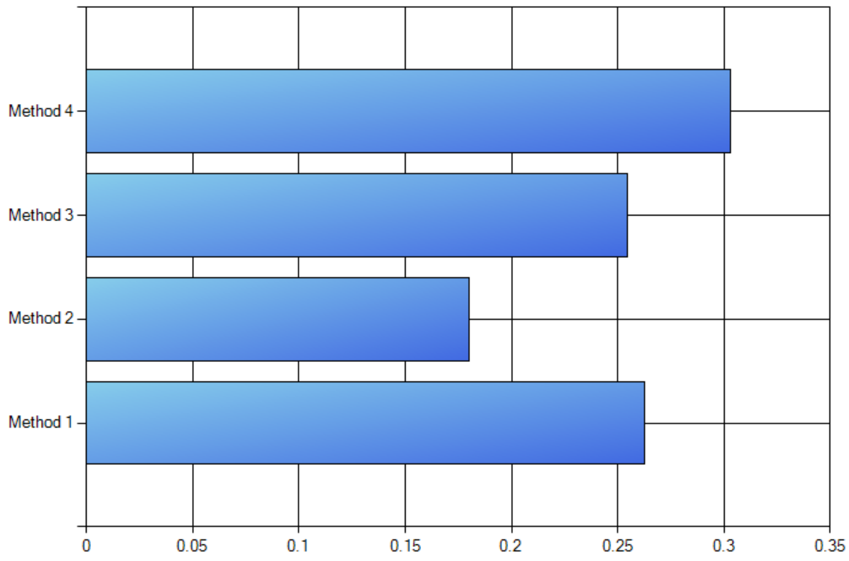


Figure 5-23 Final scores of the AHP analysis for the FFIC case study

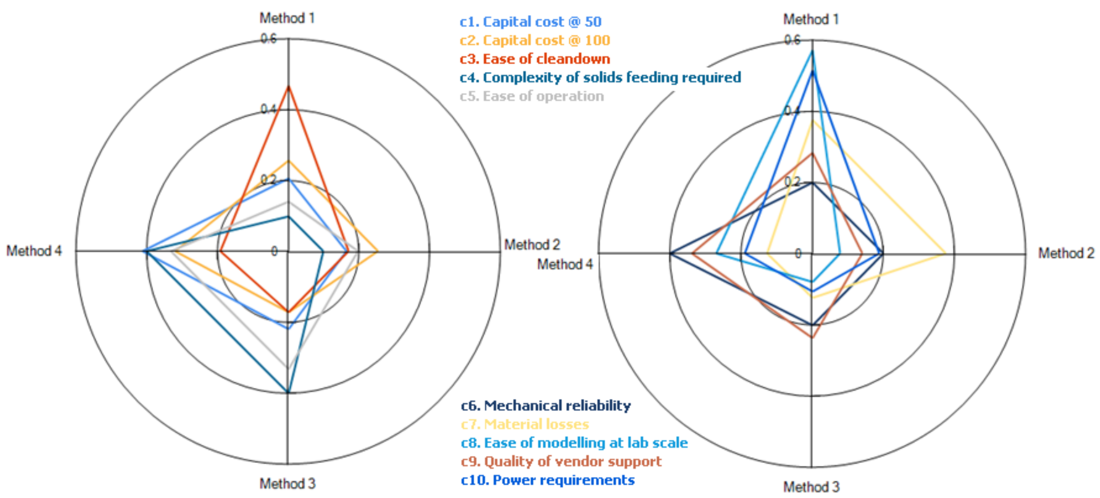


Figure 5-24 AHP decision variables for the FFIC case study

5.4.2 MARE Analysis

The MARE analysis required ten slider bar selections to determine the criteria weights (Figure 5-25). From comparing the AHP weights (Figure 5-22) and the MARE weights (Figure 5-25) it is clear that the AHP analysis had larger weights for a number of criteria including c3 ('ease of cleandown'), c4 ('complexity of solids feeding required') and c5 ('ease of operation'). In addition, the order of importance of the criteria differed, in AHP the ranking of the most influential criteria was as c5 ('ease of operation') > c3 ('ease of cleandown') > c4 ('complexity of solids feeding required') > c6 ('mechanical reliability') while for MARE it was c1 ('capital cost at

50') > c5 ('ease of operation') > c3 ('ease of cleandown') > c2 ('capital cost at 100').

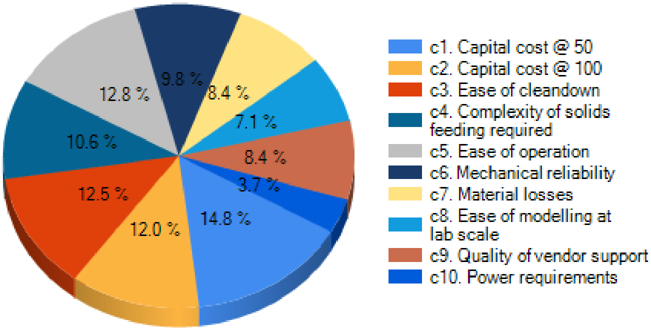


Figure 5-25 MARE criteria weights for the FFIC case study

The decision-makers chose to apply minimum and maximum values to define the uncertainty for all of the decision variables in respect to the quantitative criteria but chose only to apply one minimum and maximum selection to the decision variables for the qualitative criteria. This one selection was for method 2 in terms of c5 ('ease of operation') as shown in Figure 5-26.

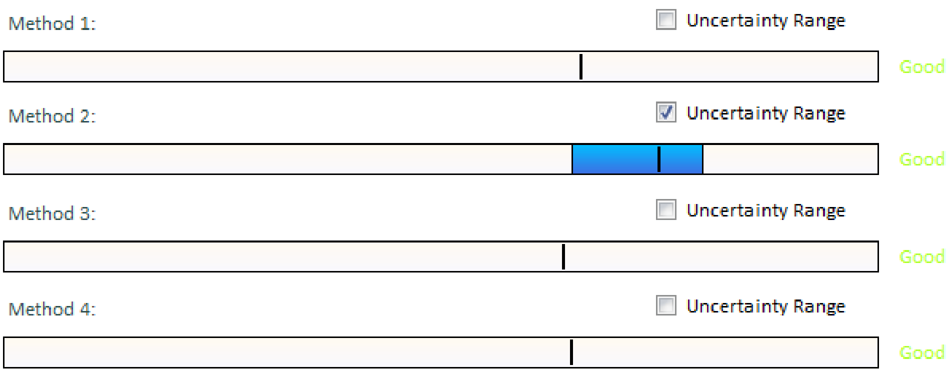


Figure 5-26 Minimum/Maximum selection for c5 ('ease of operation')

From Figure 5-26 it is clear that the most likely value of method 2 outperforms the other alternatives, however the minimum value selected is similar to the most likely values of the other alternatives, meaning in a worst case scenario, method 2 could perform similarly to methods 1, 3 and 4.

The results of the MARE analysis (Figure 5-27) indicated that method 1 was the preferred alternative due to the uncertainty range being tighter than methods 3 and 4 and the most likely value being greater in magnitude. Figure 5-28 shows that method 1 performed well in terms of c3 ('ease of cleandown'), c6 ('mechanical reliability'), c7 (‘material losses’), c8 (‘ease of modelling at a lab scale’), c9 (quality of vendor support’) and c10 (‘power requirements’).

The second best alternative in terms of most likely value was method 4. However, method 4 had a significant amount of uncertainty associated with it. In a worst case scenario, it could be the lowest performing method out of the four options. The high uncertainty in this option was a consequence of the minimum and maximum values provided for c1 (‘capital cost at 50’) and c2 (‘capital cost at 100’) as shown:

Table 5-8 Minimum and maximum values for criteria c1 and c2

		Minimum	Most Likely	Maximum
C1	Method 1	-12.5% (£350,000)	£400,000	+25% (£500,000)
	Method 2	-20% (£400,000)	£500,000	+20% (£600,000)
	Method 3	-20% (£300,000)	£375,000	+20% (£450,000)
	Method 4	**-20%** (£160,000)	£200,000	**+75%** (£350,000)
C2	Method 1	-10% (£450,000)	£500,000	+20% (£600,000)
	Method 2	-20% (£400,000)	£500,000	+20% (£600,000)
	Method 3	-33.3% (£500,000)	£750,000	+20% (£900,000)
	Method 4	**-25%** (£300,000)	£400,000	**+75%** (£700,000)

Nevertheless, as c1 (‘capital cost at 50’) and c2 (‘capital cost at 100’) are minimising criteria, desiring the lowest cost, method 4 outperformed the other methods in terms of most likely values. Method 4 also performed well in terms of c4 (‘complexity of solids feeding required’) and c6 (‘mechanical reliability’).

Method 2 had the smallest uncertainty range but was the third best alternative in terms of the most likely value. It performed well in terms of c5 (‘ease of operation’), c6 (‘mechanical reliability’), c9 (‘quality of vendor support’) and c10 (‘power requirements’). The worst performing alternative in terms of most likely value was method 3 as it performed the worst in terms of c2 (‘capital cost at 100tepa’), c3 (‘ease of cleandown’) and c7 (‘material losses’). However, method 3 did perform well in terms of c4 (‘complexity of solids feeding required’), c6 (‘mechanical reliability’) and c9 (‘quality of vendor support’).

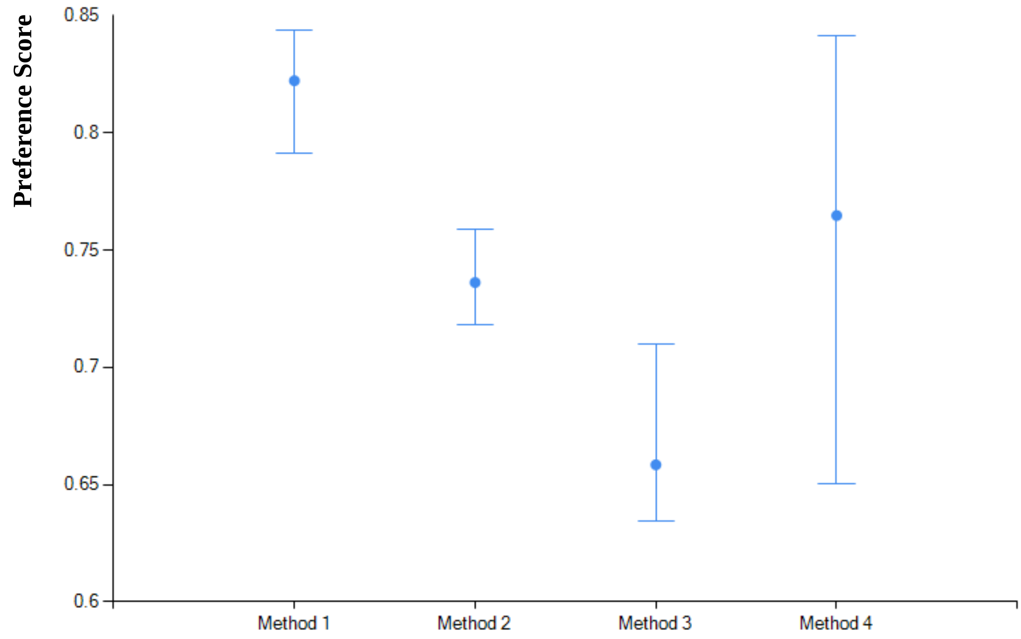


Figure 5-27 Final scores of the MARE analysis for the FFIC case study

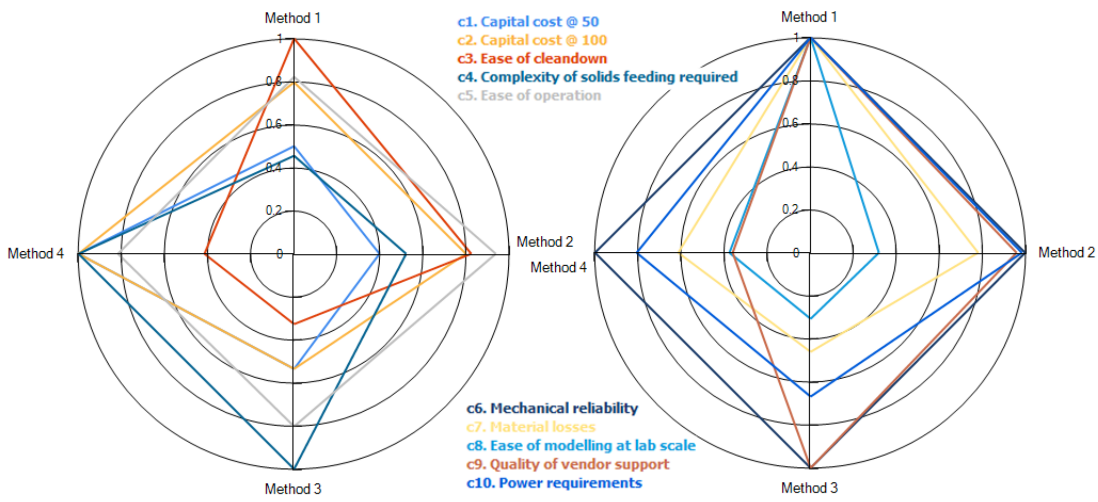


Figure 5-28 MARE likely decision variables for the FFIC case study

5.4.3 RANK Analysis

As for the MARE module, the RANK analysis required ten slider bar selections from the decision-makers to determine the criteria weights (Figure 5-29). Figure 5-29 shows that the order of the most influential criteria weights for the RANK analysis differed from that of AHP (Figure 5-22) and MARE (Figure 5-25). The four most influential criteria were the same as for MARE but in a different order as shown in Table 5-9. In AHP, c4 (‘complexity of solids feeding required’) and c6 (‘mechanical reliability') were considered more important than c1 ('capital cost at 50') and c2 ('capital cost at 100'). This discrepancy will be discussed further in Chapters 6.

Table 5-9 Four most influential criteria in AHP, MARE and RANK (FFIC)

Importance	AHP	MARE	RANK
1st	c5 ('ease of separation')	c1 ('capital cost at 50')	c1 ('capital cost at 50')
2nd	c3 ('ease of cleandown')	c5 ('ease of operation')	c2 ('capital cost at 100')
3rd	c4 ('complexity of solids feeding required')	c3 ('ease of cleandown')	c3 ('ease of cleandown')
4th	c6 ('mechanical reliability')	c2 ('capital cost at 100')	c5 ('ease of operation')

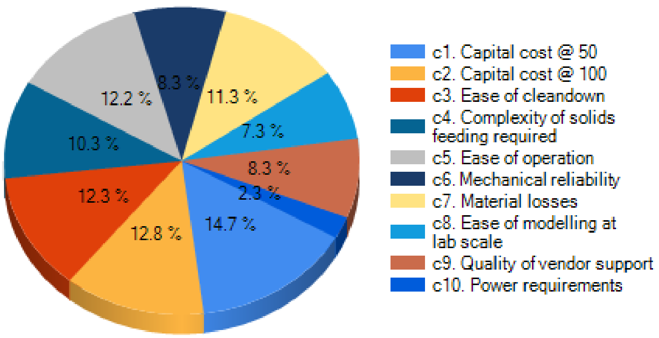


Figure 5-29 RANK criteria weights for the FFIC case study

The decision-makers used the same numerical values to determine the decision variables with respect to c1 ('capital cost at 50') and c2 ('capital cost at 100'), the two quantitative based criteria. However, the decision variables for the qualitative based criteria differed from the AHP and MARE analyses. This is discussed in the proceeding section.

The RANK tool calculated the results and displayed three rankings as shown in Figure 5-30 along with the credibility matrix in Figure 5-31.

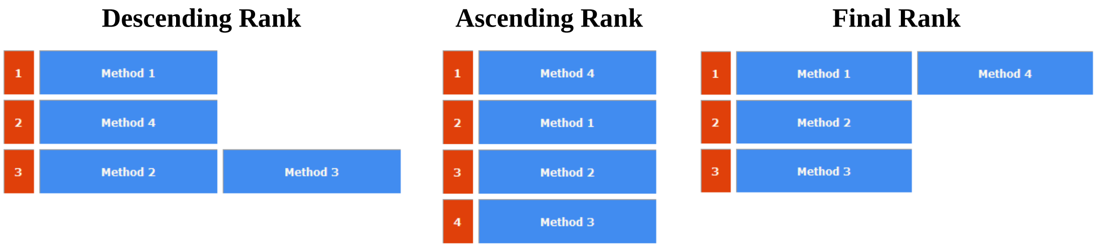


Figure 5-30 Results of the RANK analysis for the FFIC case study

The final rank shows that methods 1 and 4 are joint best alternatives. This occurred as the descending rank placed method 1 higher than method 4 while the ascending rank placed method 4 higher than method 1 making the alternative pair incomparable as shown in the credibility matrix (Figure 5-31).

	Method 1	Method 2	Method 3	Method 4
Method 1	N/A	0.985	0.897	0.000
Method 2	0.623	N/A	0.750	0.000
Method 3	0.511	0.604	N/A	0.000
Method 4	0.583	0.640	0.917	N/A

Ranked Better Incomparable Indifferent Ranked Worse

Figure 5-31 RANK Credibility index for the FFIC case study

5.4.4 Evaluation

From studying the comparisons of the criteria weights (Figure 5-32) and decision variables (Figure 5-33) it is apparent that AHP, as for the GSK case study, has emphasised a number of the decision-makers' criteria weights and qualitative decision variables.

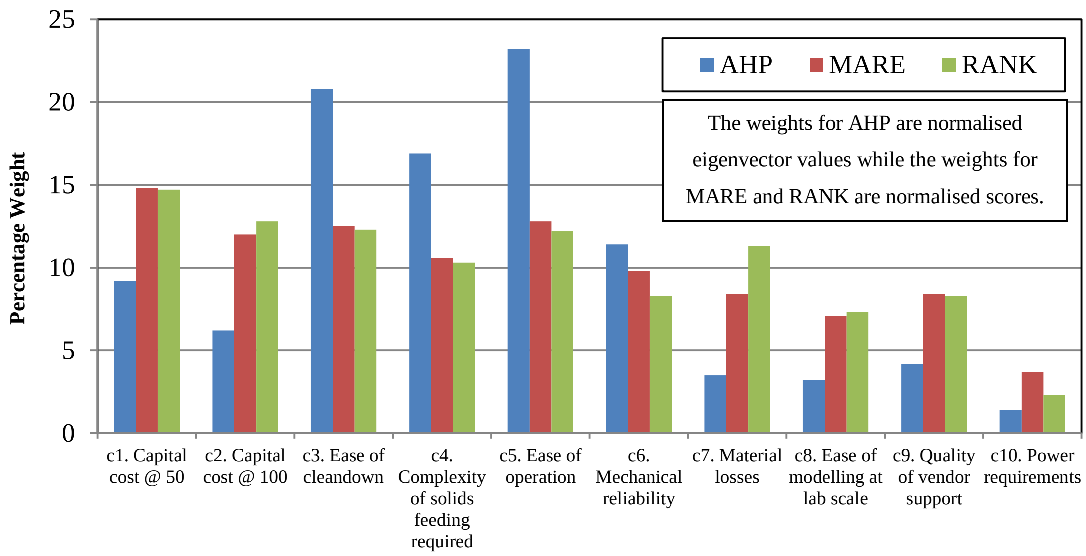


Figure 5-32 Comparison of the three analyses criteria weights (FFIC)

Figure 5-32 shows that AHP has placed greater emphasis on the weights of c3 ('ease of cleandown'), c4 ('complexity of solids feeding required'), c5 ('ease of operation') and c6 ('mechanical reliability') whilst placing less weight on the remaining criteria. However, unlike the GSK case study, the exaggerated AHP weights do not correlate to the higher weights in the MARE and RANK analyses. c1('capital cost at 50') scored the highest in terms of MARE and RANK but the same criterion was not selected as the highest weight for AHP. The main inconsistencies between MARE and RANK in terms criterion weights were in respect to c7 ('material losses'), c6 ('mechanical reliability') and c10 ('power requirements').

Figure 5-33 shows that the decision variables in relation to the two quantitative criteria (c1 and c2) were the same for the three analyses. However, inconsistencies were observed in the decision variables in relation to the eight qualitative criteria. The majority of the AHP scores differed to those for the MARE and RANK analyses. The main difference between MARE and RANK was in relation to c10 ('power requirements') but it was the least important criterion (in terms of criteria weight), so the variation in this criterion's decision variables did not have a significant impact on the results. The inconsistencies will be investigated and discussed in Chapter 6.

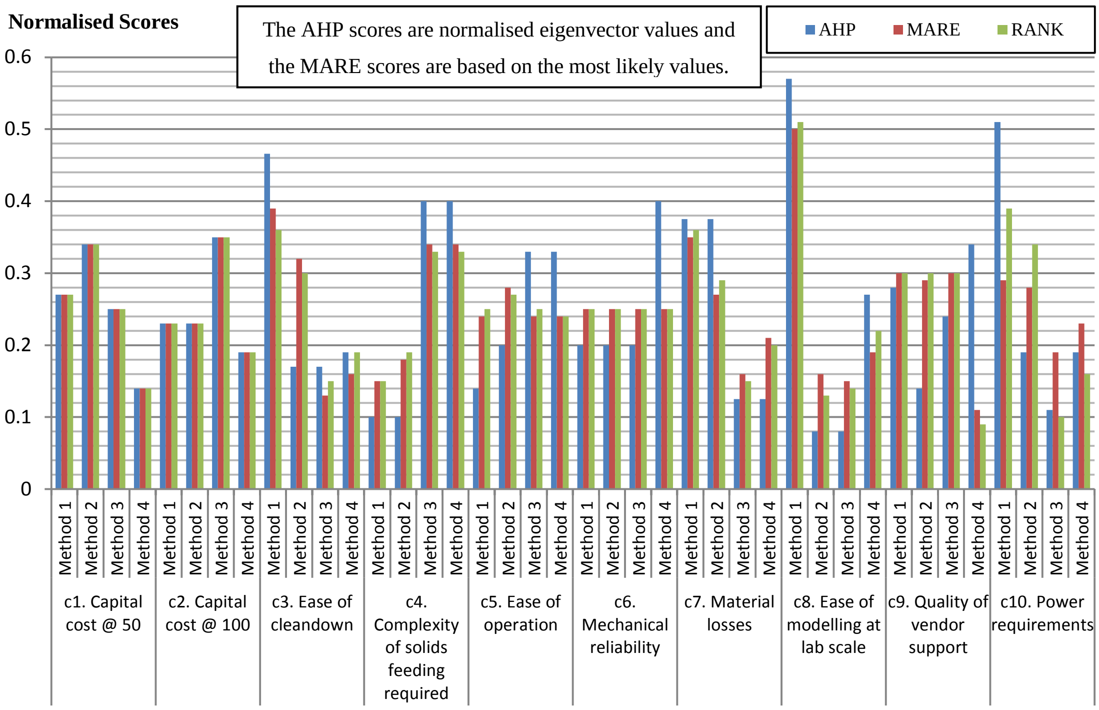


Figure 5-33 Comparison of the three analyses decision variables (FFIC)

The results of the three analyses on an ordinal scale are shown in Table 5-10. The results show that all three analyses recommended a1 and a4 over a2 and a3. However, the order of the results for the three analyses clearly differ.

Table 5-10 Comparison of the three analyses (FFIC)

	1st	2nd	3rd	4th
AHP	a4	a1	a3	a2
MARE (Most Likely value)	a1	a4	a2	a3
RANK	a1, a4		a2	a3

Table 5-11 shows the results of a sensitivity study where the specific criteria weightings for AHP, MARE and RANK have been applied to the other two methods. The results indicate that the weighting schemes have little impact on the overall results as none of the rankings have been affected by the switching of the criteria weights.

Table 5-11 Sensitivity of the criteria weights for the FFIC case study

	Weighting Scheme	1st	2nd	3rd	4th
AHP	AHP	a4	a1	a3	a2
MARE	AHP	a1	a4	a2	a3
RANK	AHP	a1, a4		a2	a3
AHP	MARE	a4	a1	a3	a2
MARE	MARE	a1	a4	a2	a3
RANK	MARE	a1, a4		a2	a3
AHP	RANK	a4	a1	a3	a2
MARE	RANK	a1	a4	a2	a3
RANK	RANK	a1, a4		a2	a3

Table 5-12 shows the results of a sensitivity study where the decision variables for AHP, MARE and RANK have been switched to the other two methods. The results show that the changes in the decision variables have a significant impact on the ordering of the alternatives.

The application of the AHP decision variables to RANK resulted in a2 becoming the worst alternative. This was a consequence of a2 scoring much lower in terms of c3, c4, c5, c6, c8, c9 and c10 in AHP (Figure 5-33). The sensitivity study (Table 5-12) also showed that the AHP decision variables placed a4 as the best alternative in all three analyses. This was due to AHP scoring a4 higher than MARE and RANK in terms of c4, c5, c6 and c9 (Figure 5-33).

Table 5-12 Sensitivity of the decision variables for the FFIC case study

	Decision Variables	1st	2nd	3rd	4th
AHP	AHP	a4	a1	a3	a2
MARE	AHP	a4	a1	a2	a3
RANK	AHP	a4	a1	a3	a2
AHP	MARE	a1	a4	a2	a3
MARE	MARE	a1	a4	a2	a3
RANK	MARE	a1, a4		a2	a3
AHP	RANK	a1	a4	a2	a3
MARE	RANK	a1	a4	a2	a3
RANK	RANK	a1, a4		a2	a3

The application of both MARE and RANK decision variables for the three analyses resulted in a similar order with the only variation being RANK placing a1 and a4 as joint best alternatives. This was caused by a1 and a4 being incomparable, as shown in RANK analysis (Figure 5-31).

The results of the sensitivity studies show that the differences in the decision variables are the cause of the differences in the orderings of the three analyses (Table 5-10).

5.4.5 Post Analyses Interview

Post analyses, the decision-maker reviewed his experiences and discussed the results. On reflection, the decision-maker preferred the MARE tool for its ability to handle uncertainty, for the unique way it supports minimum and maximum values in the quantitative input and for the visualisation of the output. In particular he liked how MARE returned "*confidence intervals*" as an output. He explained that "*the output represents reality and therefore I think MARE is good for displaying the real situation*". He also stated that "*the catch is* [with MARE that] *you might end up with multiple potential decisions still*". This statement refers to the fact that a choice still needs to be made in terms of which alternative to select as at times there are overlaps between the uncertainty ranges whilst in comparison, AHP and RANK provide a definitive result.

Considering AHP and RANK, the decision-maker favoured AHP due to "*forcing direct comparisons*" in terms of qualitative input. Furthermore, AHP is potentially the tool that can be implemented most quickly but "*for a small number of parameters only*". In terms of RANK, the decision-maker said he lacked confidence in the tool as he was "*more nervous of the outputs as AHP and MARE was more clear*".

Reflecting on the inconsistencies in the three analyses, the decision-maker observed how AHP placed considerable emphasis on a number of criteria weights and qualitative decision variables. After analysing the input in Figure 5-32 and Figure 5-33, the decision-maker stated "*MARE and RANK are pretty consistent and are probably more representative and accurate".*

From the outputs of the analyses, the decision-maker further evaluated method 4 as it had been highly ranked even though from the results of MARE, it showed much greater uncertainty. The work undertaken was unable to reveal how achievable method 4 was so in the end Fujifilm Imaging Colorants Ltd went with method 1.

5.4.6 Conclusions

The aim of this case study was to identify the best equipment option to mix a substance in the early stages of a development process. The results of MARE and RANK were similar in terms of ranking but AHP recommended a completely different order. It was recognised that AHP emphasised the decision-makers' preferences with regard to the criteria weights and decision variables. From further investigation, it was identified that the variations in the AHP decision variables were the cause of AHP providing significantly different results. Post analyses, the decision-maker selected method 1 due to the high uncertainty associated with method 4. Only the MARE method showed the uncertainty associated with method 4 and as a result, it was the favoured method for analysing this particular decision problem.

5.5 User Evaluation of the Framework

Further to the case studies, this section explores the thoughts of professionals from the chemistry-using industries that have used the ChemDecide framework. The evaluations of the users were collected in two forms, structured questionnaires and semi-structured interviews. In order to reference the views of each individual user, the users have been briefly described and numbered from 1 to 5 in Table 5-13. It should be noted that user 1 was the decision-maker of the second case study and user 2 was the decision-maker of the third case study.

Table 5-13 Industrial users who evaluated the framework

User Number	Company	Job title	Makes WPD Decisions
1	GlaxoSmithKline	Processing Engineering Manager	Yes
2	Fujifilm Imaging Colorants Ltd	Technology Manager	Yes
3	Robinson Brothers Ltd	Senior Chemical Engineer	Yes
4	Infineum	Manufacturing Technology Leader in Process Development	Yes
5	Proctor and Gamble	Senior Process Development Engineer	Yes

The conclusions of the three case studies indicated an industrial preference for the MARE methodology. However, this section will explore the particular industrial preferences in terms of the three tools' inputs, outputs, ability to handle uncertainty and analysis time. Additionally, the users' opinions regarding the ChemDecide package as a whole is explored along with proposals for future work.

5.5.1 Inputs

The favoured methods in terms of user input were AHP and MARE. None of the users opted for the qualitative or quantitative input of the RANK method. User 5 stated that he favoured AHP because "*of the feedback it provides when ranking the different options in terms of the consistency check*". He believed that the consistency check helped validate data entry in a group decision-making environment. Users 2 and 3 also preferred AHP in terms of its qualitative input. User 3 stated "*In AHP I like the comparison of individual criteria against each other, it makes you think about what criteria are really the most important*". However, in terms of quantitative input, users 2 and 3 preferred the MARE tool. Both users liked the consideration of uncertainty in the inputs which the MARE tool permitted. User 4 preferred the MARE method for both qualitative and quantitative input as it "*best allows for* *independent importance and uncertainties*". He also thought that "*AHP would be too difficult to keep track of* [in terms of] *the consistency when given a large number of criteria*". It was clear user 1 also preferred the MARE tool for both qualitative and quantitative input as it allowed "*the ability to add uncertainty*".

5.5.2 Outputs

All but one of the users favoured the MARE method in terms of output. User 3 preferred the output of AHP as it was "*clear and accurate*". The remaining users preferred the MARE tool for its ability to visualise uncertainty. User 4 described the visualisation of uncertainty as the "*uncertainty impact*" while user 2 described it as "*confidence intervals*".

5.5.3 Uncertainty

All of the users preferred the MARE tool for handling uncertainty. Both users 2 and 4 said that MARE outperformed AHP and RANK as it can display the impact of uncertainties rather than just including them in the calculations.

5.5.4 Analysis Time

The methods selected as the preferred options for conducting an analysis in terms of time were AHP and RANK. Users 2 and 3 selected AHP as the method which was quickest to implement, however, user 2 said this would only be applicable for problems with "*a small number of parameters only*". User 4 considered RANK to be the quickest method since it is "*the simplest method in terms of keeping consistency among inputs*". He explained that ensuring a level of consistency ensures meaningful results and it "*is the most time consuming step*". User 1 believed that all of the analysis methods took a similar time to conduct an analysis.

5.5.5 Overall Evaluation

All except user 4 stated that they will use the ChemDecide decision tools again for future problems. User 4 explained "*for most of the decisions that we need to make we would use a simple spread sheet for the decision making process and something more complex for understanding and prioritizing the activities to work in each of the options - ChemDecide seems to sit in between these two needs*".

In contrast, user 1 stated "*with a bit of discipline,* [ChemDecide] *might be a standard tool we could use*". Further to this, user 1 explained that he had uniquely benefited from the software's decision recommendations while also finding value in:

1. "*The way* [the tools] *led you though a structured discussion* [(in a group decision-making context)], *it was very logical*".
2. "*The way* [the tools] *got you to document what you were doing… it was nice to get a report out at the end*".

User 5 agreed with the first point, stating "*I appreciate the tools as they try to make the discussion amongst the team less driven on opinion …* [the tools] *force the team to justify their opinions using data*".

Users 3 and 4 also agreed with the second point with user 3 stating "[the tools] *could be invaluable when reviewing a process 5 or 10 years later when corporate memory is hazy*".

5.5.6 Future Requirements

Only two users provided suggestions for further requirements to the ChemDecide tools:

1. User 1 requested the capability to record decision solutions at certain times throughout product and process development so a history of solutions can be collated and used in subsequent studies. This would be of benefit to corporate memory.
2. User 2 requested that the tools be developed as one software programme. This would involve merging the common inputs for all three decision analysis modules and providing multiple outputs in a singular software interface.

5.5.7 Conclusions of the User Evaluation

It is evident that the MARE method has been favoured over AHP and RANK by the industrial users for a number of its features including the ability to visualise uncertainty and handle multiple quantitative inputs. However, the users' are not in agreement that MARE is the best method in all the categories discussed. In particular, MARE was not recognised for performing well in terms of analysis time. The implications of the users' evaluations on the ChemDecide framework will be discussed in Chapters 6 and 7.

5.6 Conclusions

This chapter presented three industrial decision-making case studies as well as five user evaluations of the framework. Each of three case studies considered a decision problem at different stages in the Whole Process Design (WPD) activity (see section 3.3.2). The goal of the initial case study was to recommend a route to synthesise a chemical (route selection stage), case study two's objective was to propose a degasification methodology for a new process (process development stage) and the final case study was to select the preferred equipment to mix a substance (flow sheet design stage).

A number of outcomes were identified from analysing the case studies and users' evaluations:

1. The Robinson Brothers case study demonstrated that with identical data, the three analysis methods recommended the same order of results. This supported the claims of Huang et al. (2011).
2. The GSK and FFIC case studies revealed that AHP emphasised a number of criteria weights and qualitative decision variables. All pairwise comparisons input by the decision-making team were mathematically consistent. Therefore, the emphasised scores, in relation to MARE and RANK, were a consequence of the unique way AHP calculated the scores. The decision-maker from GSK stated that the scores highlighted in AHP represented his preferences while the decision-maker from FFIC stated the similar scores of MARE and RANK represented his preferences.
3. Although the qualitative input methods for MARE and RANK are identical, the GSK and FFIC case studies revealed differences in the criteria weights and qualitative decision variables.
4. In the GSK and FFIC case studies, the ability to visualise the uncertainty of the different alternatives by applying the MARE method guided the decision-makers' choice.
5. The recommended alternative for all three case studies matched the alternative that had been selected a priori based on intuition. This indicates that for the three case studies discussed, system 2 (a structured decision analysis) has corresponded to the gut feeling of system 1 (section 2.3.1).

6. AHP and MARE were the recommended tools for the Robinson Brothers case study while MARE was the favoured tool for the GSK and FFIC case studies.
7. The MARE method was favoured by the industrial users for a number of its features including the ability to visualise uncertainty and handle multiple quantitative inputs. However, The MARE method was not recognised for performing well in terms of analysis time.

These outcomes yield a number of questions that will be examined in the subsequent chapter:

RQ7: What is the source of the inconsistencies in the GSK and FFIC case studies?

RQ8: Could the decision-makers' intuition have influenced the final decision results?

RQ9: Would the employment of the users' further requirements in section 5.5.6 instigate any theoretical or implementation challenges?

By addressing these questions, RQ1 can be re-examined in Chapter 7:

RQ1: What is the most effective way to support decision-making in whole process design?

"Sometimes, in order to make a decision, you need to decide on what is good enough rather than necessarily what is best" **Camilla Toulmin** (2010)

6 Case Study Discussion

6.1 Introduction

This chapter presents a discussion centred on three questions that arose from the conclusions of Chapter 5:

RQ7: What is the source of the inconsistencies in the GSK and FFIC case studies?

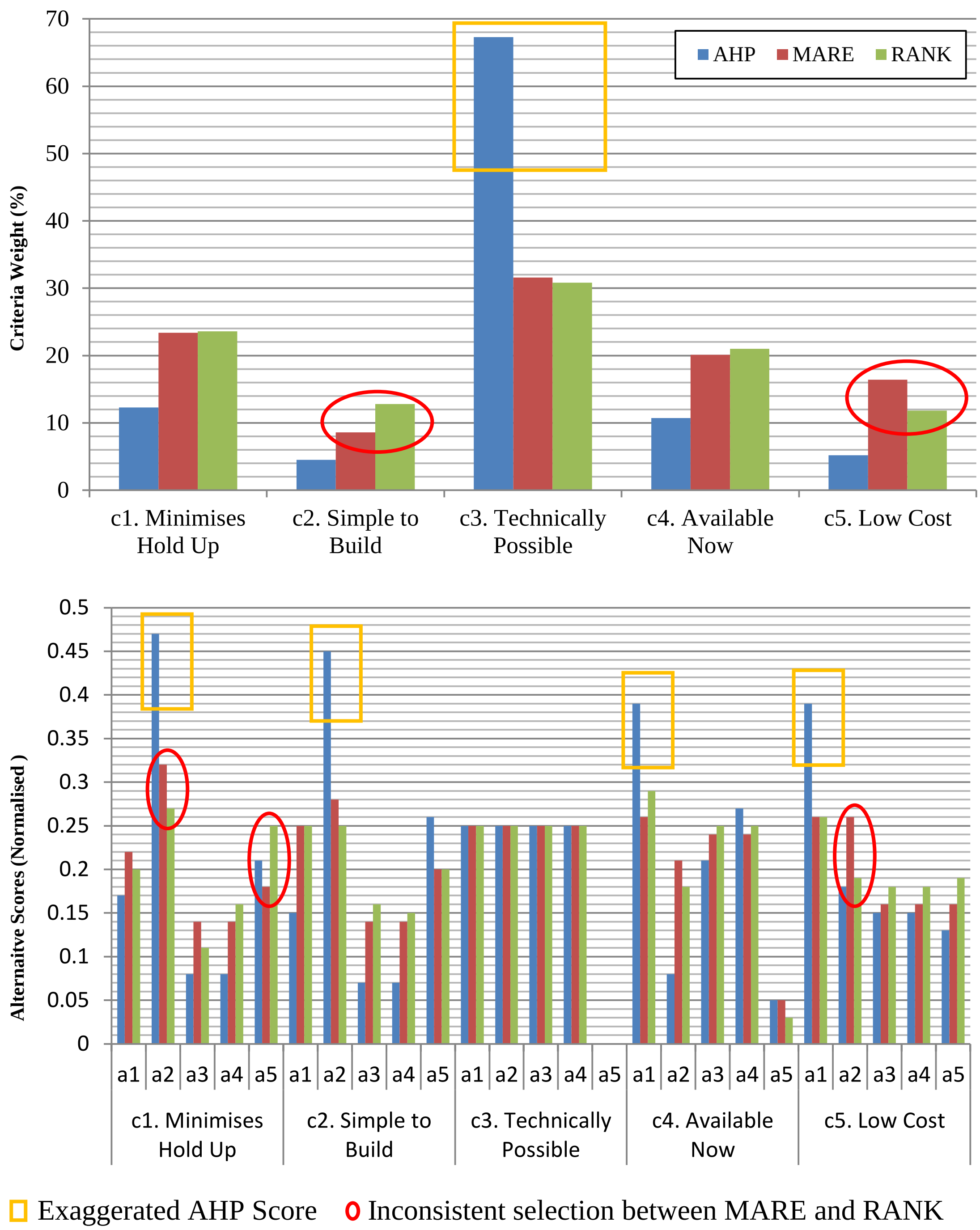
RQ8: Could the decision-makers' intuition have influenced the final decision results?

RQ9: Would the employment of the users' further requirements in section 5.5.6 instigate any theoretical or implementation challenges?

Each of the three questions will be evaluated independently using the findings from the previous chapters in relation to proposed theories and to the scientific literature considered.

6.2 Source of the inconsistencies in the case studies

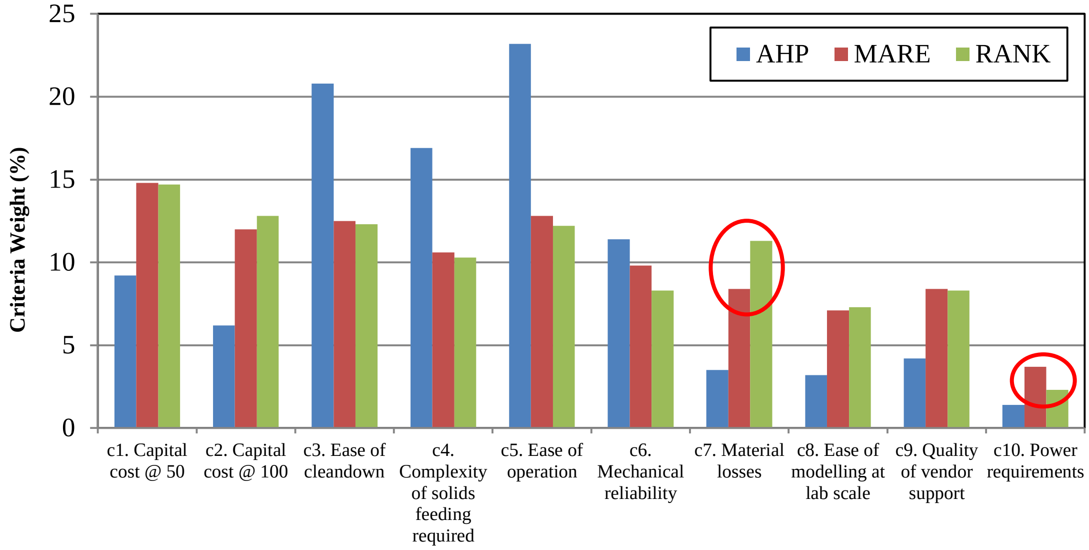
Chapter 5 presented industrial decision case studies from GlaxoSmithKline (GSK) and Fujifilm Imaging Colorants Ltd (FFIC) that were conducted by teams internal to each of the organisations. Each case study presented one decision problem that was evaluated using three analysis tools (AHP, MARE and RANK) introduced in section 4.4. An evaluation of the results for each of the analyses with respect to the two case studies identified a number of inconsistencies in the criteria weights and in the qualitative decision variables. The quantitative decision variables remained constant and thus consistent for all of the analyses. The results and inconsistencies for both the GSK and FFIC case studies are shown in Figures 6-1 and 6-2 respectively. Both figures clearly show that the qualitative weights and scores for the AHP analyses were significantly different to the MARE and RANK analyses. The dissimilar input (pairwise comparisons) of AHP could account for this. However, the significant variation in AHP in comparison to using the MARE and RANK tools may be due to the scale of the pairwise selections, this concept is discussed in section 6.2.1.

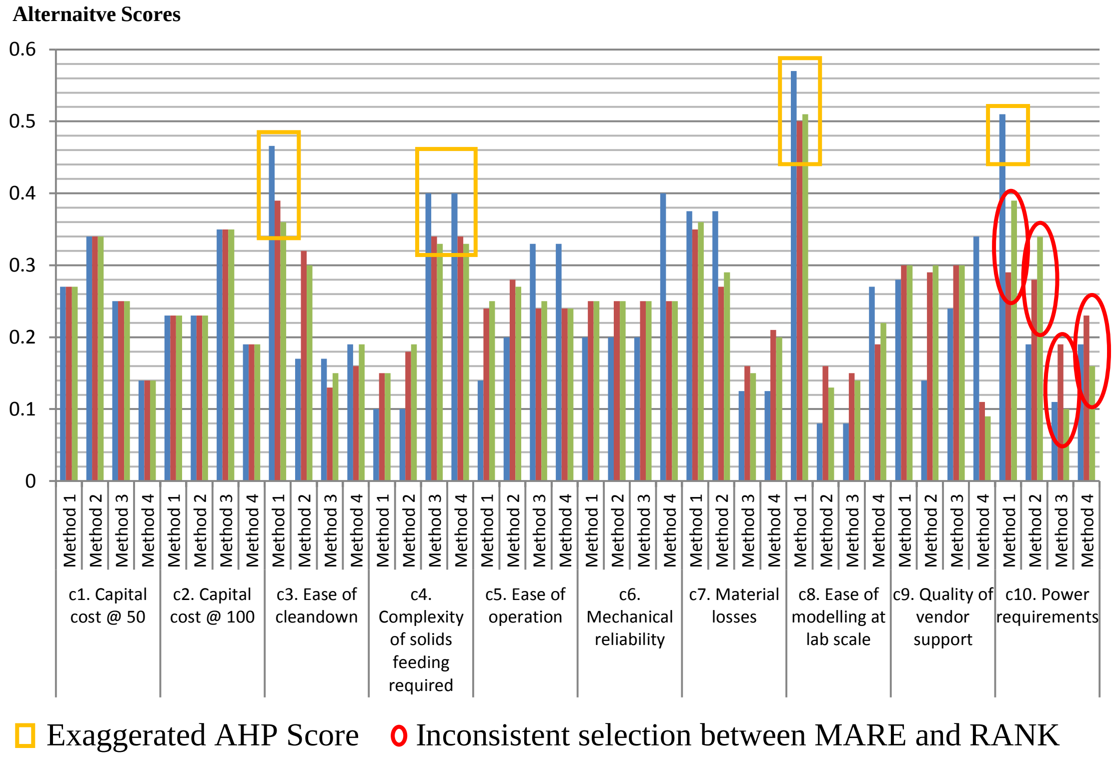


Analyses Results

	1st	2nd	3rd	4th	5th
AHP	a2	a1	a4	a3	a5
MARE (Most Likely value)	a2	a1	a4	a3	a5
RANK	a1	a2	a4	a3	a5

Figure 6-1 Results and inconsistencies in the GSK case study





Analyses Results

	1st	2nd	3rd	4th
AHP	a4	a1	a3	a2
MARE (Most Likely value)	a1	a4	a2	a3
RANK	a1, a4		a2	a3

Figure 6-2 Results and inconsistencies in the FFIC case study

As previously discussed, the MARE and RANK analyses shared identical input controls for qualitative data entry, thus their selections should have been comparable. However, Figures 6-1 and 6-2 show a number of inconsistencies between each of these analyses. Two different interpretations of how this could have occurred are discussed in sections 6.2.2 and 6.2.3.

6.2.1 Pairwise selection scale

The results of the GSK case study (Figure 6-1) clearly showed that the AHP method has placed greater emphasis on all of the better performing criteria weights and qualitative decision variables with respect to the MARE and RANK tools. This resulted in the average and lower performing criteria weights and decision variables receiving lower preferences with respect to MARE and RANK. The results of the FFIC case study (Figure 6-2) also showed a number of similar "exaggerated" qualitative decision variables using the AHP method. However, some of the preferences that dominated did not correlate to the highest performing criteria weights and decision variables in the MARE and RANK analyses.

The emphasis on the criteria weights and decision variables which were highly weighted occurred despite the fact that all of the decision-makers' pairwise comparisons were mathematically consistent. This was confirmed by the consistency ratio (CR) being below 0.8 in all of the pairwise comparison sets in both case studies (CR is discussed in Chapter 4). Therefore, either the decision-makers' knowingly placed emphasis on their preferences or there are inaccuracies in the 1-9 scale and definitions proposed by Saaty (1980):

Table 6-1 Scale of the AHP Method (Saaty, 1980; Saaty & Vargas, 2012)

Scale	Verbal Expression	Explanation
1	Equal importance	Two activities contribute equally to the objective.
3	Moderate importance	Experience and judgment slightly favour one activity over another.
5	Strong importance	Experience and judgment strongly favour one activity over another.
7	Very strong importance	An activity is favoured very strongly over another.
9	Extreme importance	The evidence favouring one activity over another is of the highest possible order of affirmation.
The values of 2, 4, 6 and 8 are compromises between the previous definitions.		

The 1-9 scale and verbal expressions proposed by Saaty (1980) in Table 6-1 suggests a relationship with equal dispersion between the scale values. Consequently, the control developed for pairwise comparison input in the AHP tool was a slider bar with equal distances between each scale selection as shown in Figure 6-3 and Appendix B. However, Salo and Hämäläinen (1997) identified that there is an uneven dispersion of values in the AHP selection scale proposed by Saaty (1980).

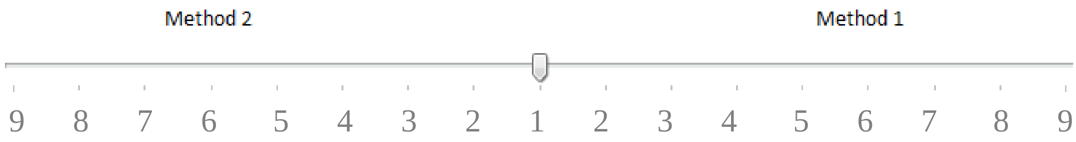


Figure 6-3 Input of pairwise comparisons in the AHP tool

They concluded that the difference in selecting between the scale of 1 and 2 is 15 times greater than the difference in selecting between the scale of 8 and 9 (Figure 6-4). This indicates that Saaty's scale (Saaty, 1980) is accountable for the overemphasised criteria weights and decision variables in the GSK and FFIC case studies.

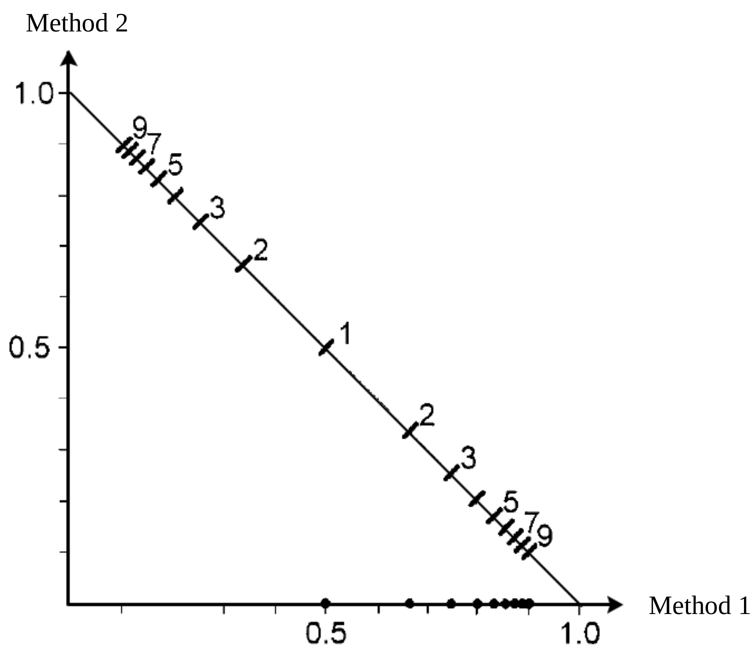


Figure 6-4 Dispersion of preferences in Satay's scale (Salo & Hämäläinen, 1997)

One solutuion to correct the slider bar in Figure 6-3 would be to modify the spread of selections to match the actual range of preferences in AHP (Figure 6-4). Another solution, proposed by Salo and Hämäläinen (1997), is to use balanced scales (Figure 6-5). For example, in Figure 6-5, the scale of 1, 1.22, 1.5, 1.86, 2.33, 3, 4, 5.67, 9 provides the balanced over [0.1, 0.9] preferences while a scale of 1, 1.27, 1.62, 2.09, 2.78, 3.86, 5.8, 10.3, 33.3 achieves the balanced over [0.0, 1.0] preferences. These scales would ensure an even dispersion of preferences that will subsequently provide uniform selections. However, Salo and Hämäläinen (1997) recognised that if a balanced scale is utilised, the consistency values which are derived from random judgements (section 4.5.2.2), would need to be recalculated in the same way as Saaty (1980) to allow for an accurate representation of the consistency ratios.

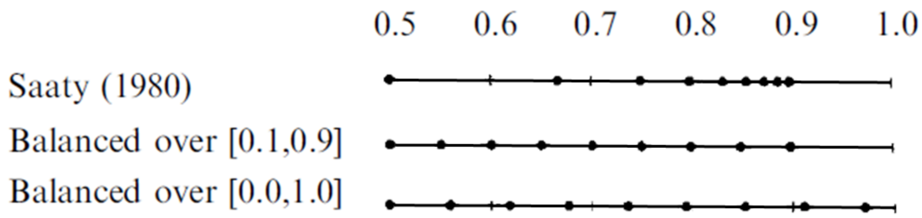


Figure 6-5 Dispersion of preferences in balanced scales (Salo & Hämäläinen, 1997)

Through an experiment investigating the interpretation of verbal statements, Salo and Hämäläinen (1997) identified that the balanced scales in Figure 6-5 outperform the scale proposed by Saaty (1980) in respect to "*capturing the subject's understanding of verbal expressions*". However, it is difficult to set a value which relates to the general interpretation of a verbal expression. For example, one person may consider 'moderately more important' as 2.5 or a 4 in a scale between 1 and 9 while Saaty's interpretation is a 3. Such differences make achieving a set of consistent selections using a pairwise scale very challenging.

It is evident therefore from the work of Salo and Hämäläinen (1997) that Saaty's scale (Saaty, 1980) in the AHP method is the primary cause for the inconsistency with regard to the over and under emphasis of the criteria weights and decision variables in terms of the MARE and RANK analyses. Nevertheless, further work is needed to understand and develop a numerical and verbal scale to accurately define selections of pairwise comparisons which will satisfactorily represent the majority of users' preferences.

6.2.2 Importance and Uncertainty

Although the input controls for MARE and RANK are identical, in both the GSK and FFIC case studies there were a number of inconsistences between the two analyses. These are shown in Figure 6-1 and Figure 6-2 respectively. In the GSK case study, it was clear that c2 (‘simple to build’) and c5 (‘low cost’) had the most significant variation in terms of the criteria weights. These criteria were also the least important for all three analyses. Correspondingly in the FFIC case study, the least important criterion c10 (‘power requirements’) also showed significant variation. However, in the FFIC case study, there was also an average performing criterion c7 (‘material losses’) that showed a high amount of variation between the MARE and RANK analyses.

For the decision variables in the GSK case study, three major inconsistencies were identified between the MARE and RANK analyses. These were the alternatives a2 (membrane) and a5 (ultrasonic) with respect to c1 (‘minimise hold up’) and a2 (membrane) in terms of c5 (‘low cost’). Coincidentally, a2 (membrane) and a5 (ultrasonic) were the alternatives with the largest uncertainty ranges as shown in Figure 5-15. In terms of the decision variables in the FFIC case study, the four major inconsistencies between MARE and RANK were for all four of the alternatives with respect to c10 (‘power requirements’). As mentioned previously, c10 was the least important criterion.

Together these findings indicate that the inconsistency of a qualitative selection between decision analyses is linked to the importance and uncertainty of that selection. In terms of uncertainty it is understandable that a decision-maker may provide inconsistent selections between analyses as they have limited information to define their preference. Furthermore, it is plausible to comprehend that a decision-maker has provided an inconsistent selection as they perceive the selection to have little impact on the decision itself. However, to gather accurate recommendations from a structured decision analysis, it is vital that decision-makers select all their preferences carefully.

6.2.3 Attention and Effort

The FFIC case study demonstrated a large scale decision problem with a significant number of criteria involved in making the decision. The size of the problem necessitated the decision-makers to consider a number of qualitative preferences which required a significant amount of time and effort. Figure 6-2 shows that the majority of the inconsistencies in this case study occurred at the end of the decision-modelling process, i.e. the decision variables in respect to c10 ('power requirements'). These inconsistencies could be due to the tiredness and lower mental acuity of the decision-maker causing a lower level of attention due to the intricacies of the decision problem itself. Vohs et al. (2005) refers to this condition as decision fatigue.

Vohs et al. (2005) stated that "*choice, to the extent that it requires greater decision-making among options, can become burdensome and ultimately counterproductive*". They argue that making multiple choices requires effort, exhausts self resources and thus impairs self-regulation. They also stated that "*the most advanced form of* [decision-making] *involves weighing information about currently available options to select the option that seems most promising*". This statement clearly describes the task of conducting a structured decision analysis. Through a series of experiments with undergraduate students, Vohs et al. (2005) found that "*self-regulation was poorer among those who had made choices than among those who had not*". Therefore it is plausible that in a larger decision problem (such as the FFIC case study) inconsistencies could occur at the end of the analysis due to prolonged attention and mental effort causing decision fatigue.

6.3 Impact of Intuition on the decision results

In section 2.3.1, the ideas of Kahneman (2011) regarding system 1 (intuition / gut instinct which is automatic) and system 2 (deep thought / contemplation that requires time and effort) thinking were introduced. The structured decision analyses in the ChemDecide software accounts for system 2 thinking by requiring the decision-makers to deeply evaluate their problem by expressing qualitative and quantitative information. The decision structuring tool records the decision-makers instinctive choice prior to each analysis which accounts for system 1 thinking. In both the GSK and FFIC case studies, the alternative chosen based on intuition was the same as the recommendations given from the structured decision analyses. This section examines whether the intuition option selected in the problem structuring phase of the decision-making process impacted on the choices made in the structured decision analysis phase.

Potentially by asking the decision-makers to indicate their intuition before the analysis, one alternative will be more prominent in the decision-makers' cognitive thought process during the analysis. This could potentially create bias for when the decision-makers provide their qualitative (subjective) preferences. However, Gigerenzer (2007) stated that "*Gut feelings … appear quickly in conciousness, we do not fully understand why we have them*". This statement suggests that intuition is instinctive and involuntary and thus would most likely be considered in the decision-making process.

For example, if asked to research how many miles are between London and Paris, instinctively one will (without knowing the answer) estimate a value or at least define a range of values cognitively before investigating the answer.

It can thus be stated that intuition and a structured decision analysis should not be considered as two competing tasks. Instead, a decision analysis should be considered as an extension of intuition. Indeed, Kahneman (2011) stated that "*System 2* [(a structured decision analysis)] *articulates judgements and makes choices, but it often endorses or rationalizes ideas and feelings that were generated by system 1* [(intuition)]".

An explanation as to why the decision-makers' intuition in the two case studies matched the recommendations of the structured decision analysis may be that the decision-makers were experienced professionals who used their expert intuition to guide their intuitive selection. Nevertheless, as identified in the example of judging the distance between London and Paris, intuition (including expert intuition) fails to consider quantitative or statistical data (Kahneman, 2011). This information has to be collected and analysed, typically after one makes an intuitive selection in terms of the decision. Therefore, with regard to the case studies, the selections made using intuition are based solely on previous experiences and knowledge, ignoring precise data in terms of cost, time, and resources for example. Furthermore, the intuitive choices provided no justification for selecting a particular alternative. In contrast, the structured decision analysis in the ChemDecide framework allows the decision-makers to record and explain the rational basis behind each of their selections. This can be used for future reference or for corporate memory.

In conclusion, the intuitive recommendation provided in the problem structuring phase could have influenced the results of the analyses. However, intuition is considered as instinctive and involuntary. Without requesting an intuitive response, the decision-makers will still consciously or subconsciously have a favoured alternative. This should not be considered as a limitation but instead as an advantage as expanding on and/or challenging intuition should deliver a more structured and explicable decision.

6.4 Theoretical and implementation challenges from the users requirements

The ChemDecide framework was initially developed with the purpose of identifying which analysis tools were the most effective for decision-making in WPD. This constrained the framework design with each individual software tool sharing similar interfaces. This section explores the theoretical and implementation challenges of fulfilling two recommendations from industrial users as discussed in section 5.5.6:

6.4.1 Recommendation 1: Records of solutions at different times throughout product and process development

A user requested the ability to record decision solutions at different points throughout product and process development so that an event history could be compared and contrasted. This would benefit decision-makers by allowing them to accumulate corporate memory that could be used to evaluate future projects at particular stages or gates. At present the tools allow for a sensitivity analysis which permits the decision-makers to modify their previous input to evaluate a new scenario. The new scenarios can be saved for review or future evaluation but it is not possible to compare more than one model at any one time.

There are two implications in adopting the proposal. Firstly, decision files that incorporate multiple decision models will need to store more data. Secondly, it will be challenging to develop an interface that can handle and present multiple decision outcomes. Clearly, the number of decision outcomes considered corresponds to the complexity of the interface. If 10 models are considered, then the outcome of 10 decisions needs to be displayed simultaneously within the confinements of the user's screen resolution.

A solution to this problem may be to develop a standalone tool that can be used to load a number of past decision models for comparison. The advantage of a standalone tool is that the interface can be designed solely for the task of decision model comparison instead of combining the interface with the structured decision analysis.

6.4.2 Recommendation 2: Combine the four tools into a single software application

A second recommendation was for the the tools in the ChemDecide framework to be built into one single software solution. The advantage of this is that the common inputs of the three analysis tools would be merged. This would save the decision-maker from re-entering information while making it easier to compare the results of the three analyses as the recommendations would be displayed in a single software interface. Limitations are also associated with this proposal. Firstly, integrating the problem structuring tool with the decision analysis tools may result in the rank reversal fault in AHP to occur. Segregating the problem structuring from the analysis ensures the decision model is not modified after preferences are added which is the cause of rank reversal in AHP (section 4.5.1). Furthermore, the input of criteria weights and decision variables with respect to the qualitative criteria in AHP is different to the MARE and RANK analyses. Therefore, the decision-maker will still need to provide pairwise comparisons for AHP alongside the direct slider bar input of MARE and RANK.

Another limitation of a single software framework is that some decisions are better solved with specific analysis methods. For example, AHP does not have the capability to represent uncertainty, so for problems with high levels of uncertainty, MARE or RANK should be utilised as opposed to AHP. Likewise, for smaller problems, a number of decision-makers preferred the subjective pairwise input of AHP over MARE and RANK (section 5.5.1). Further advantages and limitations of each method will be discussed in section 7.2. However, supposing that one method is best for addressing a particular problem, requiring the decision-maker to input method specific inputs such as pairwise comparisons for AHP, minimum and maximum values for MARE and threshold values for RANK, may consequently be more time consuming than using separate software tools.

Advantages and limitations aside, the main challenge with developing a single software solution instead of separate tools is the interface design. Not only are multiple inputs required to satisfy the input requirements of the three analysis tools but three contrasting outputs also need to be conveyed to the user. With the space restrictions of a singlescreen at a standard resolution, designing an intuitive interface that will support multiple inputs and outputs is challenging.

6.5 Conclusions

This chapter identified that inconsistencies occurred in the case studies as a result of the input scale of the AHP tool and the importance/uncertainty of independent selections. Furthermore, evidence suggests that decision fatigue can account for inconsistencies in a large scale decision problem with a high number of criteria and alternatives.

This chapter also revealed that an analysis influenced by intuition is advantageous, as expanding on and/or challenging intuition can deliver a more structured and coherent decision result.

Lastly, the chapter discussed two recommendations from industrial users. Both amendments would benefit the end user. However, both ideas require further work as the implementation of both concepts would be challenging in terms of the user interface design.

The following chapter concludes the thesis by re-examining RQ1:

RQ1: What is the most effective way to support decision-making in whole process design?

"An organization is a factory that manufactures judgements and decisions. Every factory must have ways to ensure the quality of its products in the initial design, in fabrication and in final inspections."

Nobel Prize Winner, **Daniel Kahneman** (2011)

7 Conclusions

7.1 Introduction

This chapter concludes the thesis by returning to the initial research question:

RQ1: What is the most effective way to support decision-making in whole process design?

Subsequently, the thesis contributions, publications, theoretical contributions and conclusions are summarised, followed by a description of future work.

7.2 Discussion

The overarching aim of this thesis was to identify the most effective way to support decision-making in Whole Process Design (WPD). Chapter 3 identified through interviews and questionnaires that industry requires a decision-making solution for WPD that can be used rapidly for complex decisions using a mix of qualitative and quantitative data under uncertainty.

It was identified from the questionnaires that professionals from the chemical-using industries have applied the Weighted Sum Method (WSM) in Microsoft Excel for structured decision-making. However, the WSM is incapable of handling problems with multiple scales and cannot directly account for uncertainty. Consequently, the Multi-Attribute Range Evaluations (MARE) technique was proposed in Chapter 4. This approach applies a global sensitivity analysis to the WSM to quantify the uncertainty present during particular selections. The output of MARE provides a solution which allows the user to visualise uncertainty by displaying the most likely value, maximum value and minimum value for each alternative.

Chapter 2 discussed a number of alternative techniques that can be utilised for decision-making, with the most widely applied methods being Multi-Criteria Decision-Making (MCDA) methods. Within this group of methods, it was identified that Multi-Attribute (MA) and Outranking methods would be the most appropriate for solving WPD decisions. This was a consequence of the MA and outranking methods being capable of handling qualitative and quantitative information and uncertain selections. Within the group of MA methods, the Analytic Hierarchy Process (AHP) was identified as the most commonly applied technique in the literature. Within a select group of outranking methods, Salminen et al. (1998) identified ELECTRE III (RANK) as the best method as it can directly model uncertainty using threshold values.

The performance of the MARE method was evaluated by developing a framework that utilised AHP, MARE and RANK. The framework, ChemDecide, comprises of four software tools, three relating to the analysis methods and the forth for problem structuring. Each analysis tool has its own advantages and limitations. AHP utilises pairwise comparisons for qualitaive data input but does not handle uncertainty directly. RANK handles uncertainty through the use of pseudo criteria (section 2.2.5.1) but is a relatively complex method and may not provide results in the form of a complete ranking (section 4.5.2.4). MARE visualises the impact of uncertainty with uncertainty ranges and is relatively uncomplicated however, the output may require further deliberation from the decision-maker (section 5.4.5).

The output of MARE can be considered as a limitation if the decision-maker wants an unambiguous single numerical result (in contrast to AHP and RANK). However, MARE is able to present the uncertainty associated with each option. This represents the true situation of each alternative and consequently MARE could be considered to provide a more informative result than AHP and RANK.

In the GlaxoSmithKline (GSK) and Fujifilm Imaging Colorants Ltd (FFIC) case studies (Chapter 5), the output of the MARE tool directly influenced the company's choices. In the GSK study, the decision-makers selected Packed Column (a1) as their degasification methodology over the alternative Membrane (a2) as MARE identified Membrane (a2) as having greater uncertainty even though its likely value was greater than Packed Column (a1). Similarly, in the FFIC case study, the decision-makers selected Method 1 over Method 4 to mix a substance in the early stages of a development process as Method 4 exhibited greater uncertainty when the MARE tool was utilised.

The user evaluation of the analysis tools showed that all but one person preferred the MARE method in terms of output due to the visualisation of uncertainty. The user who did not prefer MARE selected AHP as they considered the result "*clear and accurate*". This indicates that this particular user preferred an unambiguous result with a single numerical output provided for each option.

The user evaluation also showed that all of the users preferred the MARE tool for handling uncertainty. However, the MARE tool was not the favoured method for some aspects. In terms of the time required to conduct an analysis, the users preferred AHP and RANK. This was a consequence of MARE requiring the input of three values for each alternative with respect to each criterion. The MARE approach necessitates only three values for uncertain selections and with the range slider bar, the input for qualitative selections is rapid and automatically valid in terms of minimum > most likely > maximum. The time required to provide qualitative input for the AHP tool is dependent on the size of the decision problem. For example, if a problem considers three alternatives, only three pairwise comparisons are required for each qualitative criterion. However, if a decision problem considers ten alternatives, thirty-five pairwise comparisons are required. The RANK tool requires one score for each alternative along with three threshold values for each criterion. Therefore, for larger problems with significant uncertainty, RANK would require the lowest number of input selections from the user. It can be stated that the number of input selections required for each analysis tool is dependent on the size of the problem and the uncertainty present. This was identified by the decision-makers of the FFIC case study (section 5.5.4).

In terms of selecting between AHP, MARE and RANK for decision-making in WPD, the choice is not straightforward. From reviewing the three WPD case studies discussed in Chapter 5, both the AHP and MARE methods were able to recommend a single best alternative. RANK failed to provide a complete ranking in the FFIC case study as it recommended two alternatives as joint best. As discussed, the MARE method, unlike AHP and RANK provides additional information regarding the uncertainty of each option along with the most likely values for each alternative. Due to the nature of WPD decisions where uncertainty is present, understanding the true situation (in regards to uncertainty) behind each decision outcome is crucial to the success of decision-making in WPD. Therefore, with the visual interpretation of uncertainty in terms of the output of MARE, it is proposed as the most effective way to support decision-making throughout WPD. Nevertheless, further investigations are still required and are discussed in section 7.5.

7.3 Thesis Contribution

In summary the main contributions of this thesis are as follows:

- An extensive literature review identified and described the most commonly applied decision-making techniques for Multi-Criteria Decision Analysis.
- A further literature review identified techniques proposed for decision-making in chemical product and process development.
- Two semi-structured interviews and two structured questionnaires identified the industrial requirements for decision-making in whole process design.
- A novel methodology, Multi-Attribute Range Evaluations (MARE), was proposed as a solution for decision-making in whole process design.
- A novel two-phase system (problem structuring then analysis) for decision-making was proposed to prevent rank reversals, ensure consistency throughout multiple analyses and to encourage the decision-maker to focus on the problem structuring process.
- A software framework (ChemDecide) was developed which contains four tools, one for problem structuring and three for analysis.
- Three industrial whole process design decision-making case studies were developed in collaboration with Robinson Brothers, GlaxoSmithKline and Fujifilm Imaging Colorants Ltd.
- Structured questionnaires and semi-structured interviews identified the thoughts of five professionals who used the ChemDecide framework.
- Inconsistencies that arose in the three industrial case studies were analysed and discussed.
- Behavioural decision-making was introduced and the idea that intuition affects a structured decision analysis was discussed.

7.4 Publications

Hodgett, R. E., Martin, E., Montague, G., Talford, M., 2012. Handling uncertain decisions in Whole Process Design. Production Planning & Control. Under Review.

Hodgett, R. E., Manipura, A., Martin, E., Montague, G., 2013. Comparison of AHP, MARE and ELECTRE III for Equipment Selection. European Journal of Operational Research. Expected Submission.

7.5 Theoretical Contributions

This thesis introduces a number of theoretical contributions and assumptions. The following of which have been discussed in detail:

- A number of theories were proposed for how the inconsistencies occurred in the industrial decision case studies presented in Chapter 5. In particular, the importance and uncertainty of independent selections, the input scale of AHP and decision fatigue are thought to be accountable for the inconsistencies identified (section 6.2).
- A theory was proposed that considers intuition to be beneficial to the decision-making process as expanding on and/or challenging intuition should deliver a more structured/coherent decision result (section 6.3).
- The majority (87%) of the industrial members questioned (section 3.3.3.3) required support for group decision-making. However, all group decision-making models suffer from intransitivity and bias from dominant members (section 2.3.2). Various theories are proposed to tackle these issues:
    - Ensuring decision-makers collectively reflect on their findings and carry out a sensitivity study will encourage silent members to voice their opinion.
    - Justifying (discussing and clarifying) each selection in the decision-making process will also encourage silent members to voice their opinion.
    - Checking for mathematical consistency in the decision-making process will insure transitivity of the decision-makers selections.

  All of the above techniques have been incorporated (where possible) into the ChemDecide framework.

One theoretical contribution relating to dynamic alternative/value focused thinking was given less coverage in the earlier chapters. This theory will be clarified and elucidated in the proceeding section.

7.5.1 Dynamic problem structuring with values and objectives

As discussed in section 2.2.2.1, various theories have been proposed to systematically guide the identification of criteria and alternatives in the decision structuring process. Alternative focused thinking refers to the process of identifying alternatives then identifying criteria. Keeney (1992) instead proposed value focused thinking which refers to the process of identifying criteria then identfying alternatives. More recently, Corner, et al. (2001) proposed dynamic decision problem structuring which is a process that cycles between value focused thinking and alternative focused thinking (Figure 7-1). The idea is that the consideration of criteria prompts creative thinking about the alternatives which in turn generates new criteria, and so on.

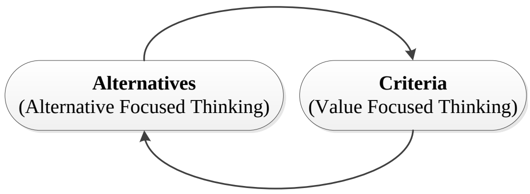


Figure 7-1 Dynamic Decision Problem Structuring (Corner, et al., 2001)

Although the dynamic decision problem structuring process "*encourages decision makers to reflect on and learn about their values and the problem context*" (Belton & Stewart, 2010), Franco & Montibeller (2009) believe that the theory lacks psychological asepects (e.g. how to instigate creativity) and group dynamics (e.g. how to identify and display complex scenarios to a group of decision-makers). Therefore, the dynamic decision problem structuring model was adapted to include two preceding steps, definition of the problem and brainstorm objectives (Figure 7-2). This model was incorperated into the decision structing software (DecisionStructure) of the ChemDecide framework (Figure 4-4).

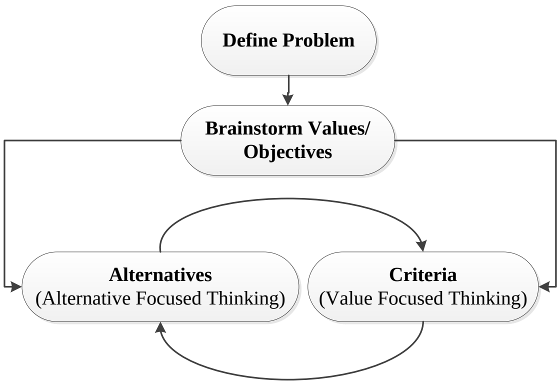


Figure 7-2 Dynamic Decision Problem Structuring with Values and Objectives

There are two advantages to the amended problem structuring model. Firstly, the define problem stage insures that the decision-makers collectively understand the problem they are trying to solve. Secondly, the brainstorm objectives and values stage permits the decision-makers to gather and discuss goals and outlooks which can be used to identify suitable alternatives and criteria. Although this model was evaluated empirically by the three industrial case studies discussed in chapter 5, it is difficult to measure the proficiency of the theory without directly comparing it to other problem structuring models.

7.6 Conclusions

In summary the main conclusions of this thesis are as follows:

- Professionals in the chemical-using industries require a system for rapidly making complex decisions with limited/uncertain information in whole process design.
- A number of techniques have been proposed for decision-making in the chemical-using industries but only three methods have been considered to address real-world problems in the literature; Analytic Hierarchy Process (AHP), Analytic Network Process (ANP) and Weighted Sum Method (WSM).
- Many professionals in the chemical-using industries use techniques for brainstorming but very few utilise methods for a structured decision analysis.
- From the WPD stages defined by Sharratt (2011), members of Britest Ltd indicated that the most commonly faced decision problem was chemical route selection.
- A newly proposed methodology, Multi-Attribute Range Evaluations (MARE), outperformed the Analytical Hierarchy Process (AHP) and ELECTRE III (RANK) in terms of handling and visualising uncertainty.
- A case study with Robinson Brothers Ltd demonstrated that with identical criteria weights and decision variables, multiple analysis methods recommend the same order of results supporting the claims of Huang et al. (2011).
- An evaluation of the inconsistencies in the GlaxoSmithKline and Fujifilm Imaging Colorants Ltd case studies identified that:

  - There is an uneven dispersion of scale values in the Analytical Hierarchy Process.
  - Decision-makers are more likely to make inconsistent qualitative selections when the choice has little impact on the decision itself or is associated with high amounts of uncertainty.
  - Decision-makers who evaluate large decision problems with many alternatives and criteria (such as the Fujifilm Imaging Colorants Ltd case study) may suffer from "decision fatigue".
- Intuition is valuable in guiding a structured decision-analysis as expanding on and/or challenging intuition can deliver a more structured and coherent decision recommendation.

7.7 Future Work

This section addresses particular areas where further research is required.

7.7.1 Further case studies

Britest Ltd intend to add the ChemDecide software framework to their collection of tools and methodologies. As a consequence of this, further case studies will be developed with the industrial members of Britest. These case studies will be used to validate the findings in Chapter 5 and assess the proposed theories in Chapter 6.

7.7.2 Guidelines for method selection

Although this thesis proposes the use of Multi-Attribute Range Evaluations (MARE) for whole process design decisions (where uncertainty is high), it is evident from the user evaluations in section 5.5 that MARE is not necessarily the best method for all decision problems. The nature of the problem, i.e. the complexity, uncertainty present, number of alternatives/criteria etc., may be used to select a particular MCDA method. This concept needs to be investigated further to see if a selection algorithm or procedure can be added after the problem structuring process and before the structured decision analysis.

7.7.3 Group decision-making

The respondents of the questionnaires in Chapter 3 acknowledged that group decision-making was a highly sought after feature in a decision-making framework for use in whole process design. The GlaxoSmithKline and Fujifilm Imaging Colorants Ltd case studies demonstrated that the ChemDecide framework can successfully be used in a group decision-making environment by one person undertaking the analysis. However, as discussed in section 2.3.2, French (2007) suggested the use of an online individual voting system in group decision-making to overcome biases. This idea needs to be investigated further and possibly implemented into the ChemDecide framework.

7.7.4 Customise the software framework

Two users requested modifications to the interface of the ChemDecide framework. These were to develop all of the four tools into a single software solution and to implement the ability to record decision solutions at different times throughout product and process development. Both of these requirements need to be investigated further to see if the amendments are possible and if they will add value to the framework.

7.7.5 AHP Scales

In section 6.2.1 it was identified that the pairwise selection scale in AHP (Saaty, 1980) was accountable for the overemphasised criteria weights and decision variables in the GSK and FFIC case studies. Salo and Hämäläinen (1997) proposed two balanced scales, balanced over [0.1, 0.9] and balanced over [0.0, 1.0], to achieve an even dispersion of preferences in the AHP method. To investigate the effectiveness of the balanced scales, the values in

Table **7-1** for balanced over [0.1, 0.9] and balanced over [0.0, 1.0] can be used instead of the values proposed by Saaty (1980) in the ChemDecide framework.
The GSK and FFIC case studies can then be re-evaluated to see if the criteria weights and decision variables of AHP (using the amended scale values) are more consistent with the criteria weights and decision variables of the MARE and RANK analyses.

Table 7-1 AHP Scale values

Saaty (1980) Scale:	1	2	3	4	5	6	7	8	9
Balanced Over [0.1, 0.9]:	1	1.22	1.5	1.86	2.33	3	4	5.67	9
Balanced Over [0.0, 1.0]:	1	1.27	1.62	2.09	2.78	3.86	5.8	10.3	33.3

7.7.6 Commercialisation

In 2011, the author of this thesis was awarded with a £3,000 enterprise grant to commercialise the ChemDecide software for use in other industries. The grant was awarded by the EPSRC and Newcastle University's Medical School. The plan is to rebrand the tools as generic decision-making solutions and licence them to companies in industries that deal with finance, consultancy and engineering.

Bibliography

Aaker, D. A., 2001. Strategic Market Management. John Wiley & Sons Inc.

Adu, I. K., Sugiyama, H., Fischer, U. & Hungerbühler, K., 2008. Comparison of methods for assessing environmental, health and safety (EHS) hazards in early phases of chemical process design. Process Safety and Environmental Protection, 86(2), pp. 77-93.

Albrecht, T., Papadokonstantakis, S., Sugiyama, H. & Hungerbühler, K., 2010. Demonstrating multi-objective screening of chemical batch process alternatives during early design phases. Chemical Engineering Research and Design, 88(5-6), p. 529–550.

Allais, M., 1953. Le comportement de l'homme rationnel devant le risque: critique des postulats et axiomes de l'Ecole Américaine. Econometrica, 21, pp. 503-546.

Anon., 1980. Procedures for performing a failure mode effect and criticality analysis (MIL-STD-1629A). Department of Defence, United States of America.

Arrow, K. J., 1963. Social Choice and Individual Values. 2nd ed. New York: John Wiley and Sons.

Bayes, T., 1763. An Essay towards solving a Problem in the Doctrine of Chance. By the late Rev. Mr. Bayes, communicated by Mr. Price, in a letter to John Canton, M. A. and F. R. S. Philosophical Transactions of the Royal Society of London, 53, pp. 370-418.

Behzadian, M., Kazemzadeh, R. B., Albadvi, A. & Aghdasi, M., 2010. PROMETHEE: A comprehensive literature review on methodologies and applications. European Journal of Operational Research, 200, pp. 198-215.

Belton, V. & Stewart, T., 2010. Chapter 8: Problem Structuring and Multiple Criteria Decision Analysis. In: Greco, M. Ehrgott & J. R. Figueira, eds. Trends in Multiple Criteria Decision Analysis. Springer, pp. 209-239.

Beni, G. & Wang, J., 1989. Swarm Intelligence in Cellular Robotic Systems. NATO Advanced Workshop on Robots and Biological Systems.

Bernard, R., 1985. Méthodologie multicritère d'aide à la décision. Economica.

Bernoulli , N. & de Montmort, P. R., 1713. Personal Communication.

Bernoulli, D., 1738. Specimen theoriae novae de mensura sortis (Exposition of a New Theory on the Measurement of Risk).

Binmore, K., 2011. Rational Decisions. Fourth Edition ed. Princeton University Press.

Blum, C., 2005. Ant Colony Optimization: Introduction and recent trends. Physics of Life Reviews, 2, pp. 353-373.

Bourguignon, B. & Massart, D. L., 1994. The Oreste method for multicriteria decision making in experimental chemistry. Chemometrics and Intelligent Laboratory Systems, 22, pp. 241-256.

Branke, J., Deb, K., Miettinen, K. & Słowi´nski, R., 2008. Preface: 4. Evolutionary Multiobjective Optimization. In: Multiobjective Optimization: Interactive and Evolutionary Approaches. Berlin: Springer, p. VII.

Brans, J. P., 1982. L’ingénierie de la décision: élaboration d’instruments d’aide à la décision. La méthode PROMETHEE. Presses de l’Université Laval.

Brans, J. P. & Vincke, P., 1985. A preference ranking organisation method : The PROMETHEE method for MCDM. Management Science, 31(6), pp. 647-656.

Brans, J. P. & Mareschal, B., 1995. The PROMETHEE VI Procedure, How to Differentiate Hard from Soft Multi-criteria Problems. Journal of Decision Systems, 4, pp. 213-223.

Brans, J. P. & Mareschal, B., 2005. PROMETHEE Methods. In: Multiple Criteria Decision Analysis: State of the Art Surveys. Springer, pp. 163-195.

Brans, J. P., Mareschal, B. & Vincke, P., 1984. PROMETHEE: a new family of outranking methods in multicriteria analysis. In: J. P. Brans, ed. Operational Research '84. North Holland: pp. 477-490.

Brent, R. J., 2006. Applied Cost–Benefit Analysis. Second Edition ed. Cheltenham: Edward Elgar Publishing Limited.

Britest Ltd, 2012. Britest Limited. Available at: http://www.britest.co.uk/

Buchanan, J. T., Sheppard, P. J. & Vanderpooten, D., 1999. Project Ranking Using Electre III. Department of Management Systems, University of Waikato.

Buzan, T. & Buzan, B., 1996. The Mind Map Book: How to Use Radiant Thinking to Maximize Your Brain's Untapped Potential. Plume.

C&EN Business Group, 2011. A Long Year of Demand Recovery, Chemical & Engineering News.

Campbell, H. F. & Brown, R. P. C., 2003. Benefit-Cost Analysis: Financial and Economic Appraisal using Spreadsheets. Cambridge: Cambridge University Press.

Cassidy, D., Gotpagar, J., Morawietz, M. & Verity, R., 2011. 2012 Chemicals Industry Perspective. Booz & Company.

Cefic, 2012. Chemicals Trends Report: Monthly summary: August 2012. Cefic, the European Chemical Industry Council.

Chakraborty, S. & Yeh, C. H., 2007. A Simulation Based Comparative Study of Normalization Procedures in Multiattribute Decision Making. Proceedings of the 6th WSEAS Int. Conf. on Artificial Intelligence, Knowledge Engineering and Data Bases, pp. 102-109.

Charnes, A. & Cooper, W., 1961. Management Models and Industrial Applications of Linear Programming. New York: John Wiley & Sons.

Charnes, A., Cooper, W. W. & Ferguson, R. O., 1955. Optimal Estimation of Executive Compensation by Linear Programming. Management Science, 1(2), pp. 138-151.

Charpentier, J. C., 2002. The triplet "molecular processes–product–process" engineering: the future of chemical engineering? Chemical Engineering Science, 57, pp. 4667-4690.

Charpentier, J. C., 2007. Among the trends for a modern chemical engineering: CAPE an efficient tool for process intensification and product design and engineering. 17th European Symposium on Computer Aided Process Engineering, pp. 1-8.

Chauhan, A. & Vaish, R., 2012. A comparative study on material selection for micro-electromechanical systems. Materials and Design, 41, pp. 177-181.

Chen, H. & Shonnard, D. R., 2004. Systematic Framework for Environmentally Conscious Chemical Process Design: Early and Detailed Design Stages. Industrial and Engineering Chemistry Research, 43(2), pp. 535-552.

Chou, S. Y., Chang, Y. H. & Shen, C. Y., 2008. A fuzzy simple additive weighting system under group decision-making for facility location selection with objective/subjective attributes. European Journal of Operational Research, 189(1), pp. 132-146.

Cleeremans, A., Waroquier, L., Marchiori, D. & Klein, O., 2009. To think or not think: A critique and reappraisal of Unconscious Thought Theory. 13th Meeting of the Association for the Scientific Study of Consciousness, Berlin, Germany., pp. 81-82.

Colorni, A., Dorigo, M. & Maniezzo, V., 1991. Distributed Optimization by Ant Colonies. actes de la première conférence européenne sur la vie artificielle, pp. 134-142.

Cooper, R. G., 2001. Winning at New Products: Accelerating the Process from Idea to Launch. 2nd ed. Basic Books.

Corner, J., Buchanan, J. & Henig, M., 2001. Dynamic decision problem structuring. Journal of Multi-Criteria Decision Analysis, 10, pp. 129-141.

Dawkins, R., 1976. The selfish gene. New York: Oxford University Press.

Dias, L. C., Costa, J. P. & Cllmaco, J. N., 1998. A parallel implementation of the PROMETHEE method. European Journal of Operational Research, 104, pp. 521-531.

Diercks, R., 2012. Outlook for Chemical Industry. DECHEMA Gesellschaft für Chemische Technik und Biotechnologie. (Society for Chemical Engineering and Biotechnology).

Dijksterhuis, A., Bos, M. W., Nordgren, L. F. & van Baaren, R. B., 2006. On Making the Right Choice: The Deliberation Without Attention Effect. Science, p. 1005.

Donaldson, C., Currie, G. & Mitton, C., 2002. Cost effectiveness analysis in health care: contraindications. British Medical Journal: Education and debate, 325, p. 891–894.

Double, J. M., 2010. Whole Process Design. University of Coimbra, Coimbra, Portugal: presentation at the EU FP7 PILLS project mid-term dissemination event.

Dorigo, M., 1992. Optimization, Learning and Natural Algorithms. PhD Thesis, Politecnico di Milano, Italy.

Doumpos, M. & Zopounidis, C., 2004. Developing sorting models using preference disaggregation analysis: An experimental investigation. European Journal of Operational Research, 154, pp. 585-598.

Dyer, J. S. et al., 1992. Multiple Criteria Decision Making, Multiattribute Utility Theory: The Next Ten Years. Management Science, 38(5), pp. 645-654.

Earnshaw, S. R., Wilson, M., Mauskopf, J. & Joshi, A. V., 2009. Model-Based Cost-Effectiveness Analyses for the Treatment of Acute Stroke Events: A Review and Summary of Challenges. Value in Health, 12(4).

Edgeworth, F. Y., 1881. Mathematical Psychics: An Essay on the Application of Mathematics to the Moral Sciences. C.K. Paul & co.

El-Mihoub, T. A., Hopgood, A. A., Nolle, L. & Battersby, A., 2006. Hybrid Genetic Algorithms: A Review. Engineering Letters, 13(2).

Federsel, H. J., 2010. How to conduct research in the pharmaceutical industry? Facing the dilemma: small, autonomous teams versus large, integrated centers. Expert Opinion on Drug Discovery, 5(9), pp. 813-818.

Federsel, H. J., 2010b. Process R&D under the magnifying glass: Organization, business model, challenges, and scientific context. Bioorganic & Medicinal Chemistry, 18, pp. 5775-5794.

Fenton, N. & Neil, M., 1999. Making Decisions: Bayesian Nets and MCDA. Centre for Software Reliability, City University London.

Figueira, J., de Smet, Y. & Brans, J. P., 2004. MCDA methods for sorting and clustering problems: Promethee TRI and Promethee CLUSTER. Université Libre de Bruxelles. Service deMathématiques de la Gestion.

Figueira, J., Greco, S. & Ehrgott, M., 2005. Introduction. In: Multiple Criteria Decision Analysis: State of the art Surveys. Boston: Springer Science and Business Media, Inc.

Fine, L. G., 2009. The Swot Analysis. Createspace.

Fogel, L. J., Owens, A. J. & Walsh, M. J., 1966. Artificial Intelligence through Simulated Evolution. John Wiley.

Franco, A. & Montibeller, G., 2009. Problem Structuring for Multi-Criteria Decision Analysis Interventions. Operational Research Group, Department of Management London School of Economics and Political Science.

French, S., 2007. Web-enabled strategic GDSS, e-democracy and Arrow's theorem: A Bayesian perspective. Decision Support Systems, 43, pp. 1476-1484.

French, S., 2009. Combining Expert Judgement – A review for decision makers. Proceedings of Subjective Bayes, Warwick 14-16 December 2009.

García-Cascales, S. M. & Lamata, T. M., 2011. On rank reversal and TOPSIS method. Mathematical and Computer Modelling, In Press.

Garey, M. R. & Johnson, D. S., 1979. Computers and Intractability: A Guide to the Theory of NP-Completeness. New York: Freeman.

Gass, S. I., 2005. Model World: The Great Debate - MAUT Versus AHP. Interfaces, 35(4), pp. 308-312.

George, E., Titchener-Hooker, N. J. & Farid, S. S., 2007. A multi-criteria decision-making framework for the selection of strategies for acquiring biopharmaceutical manufacturing capacity. Computers & Chemical Engineering, 31(8), p. 889–901.

Giannoulis, C. & Ishizaka, A., 2010. A Web-based decision support system with ELECTRE III for a personalised ranking of British universities. Decision Support Systems, 48(3), pp. 488-479.

Gigerenzer, G., 2007. Gut Feelings: Short Cuts to Better Decision Making. Viking.

Gladwell, M., 2005. Blink: The Power of Thinking Without Thinking. Allen Lane.

Grime, K., 2011. Smart R&D pays off. Chemistry and Industry, (8).

Grossmann, I. E., 2005. Challenges in the New Millennium: Product Discovery and Design, Enterprise and Supply Chain Optimization, Global Life Cycle Assessment. Computers and Chemical Engineering, 29, pp. 29-39.

Guitouni, A. & Martel, J. M., 1998. Tentative guidelines to help choosing an appropriate MCDA Method. European Journal of Operational Research, 109, pp. 501-521.

Gutjahr, W. J., 2003. A Converging ACO Algorithm for Stochastic Combinatorial Optimization. Stochastic Algorithms: Foundations and Applications, Second International Symposium, SAGA, pp. 10-25.

Harless, D. W. & Camerer, C. F., 1994. The Predictive Utility of Generalized Expected Utility Theories. Econometrica, 62(6), pp. 1251-1289.

Hey, J. D. & Orme, C., 1994. Investigating Generalizations of Expected Utility Theory Using Experimental Data. Econometrica, 62(6), pp. 1291-1326.

Holland, J. H., 1975. Adaptation in natural and artificial systems. Michigan: Ann Arbor MI: The University of Michigan Press.

Huang, I. B., Keisler, J. & Linkov, I., 2011. Multi-criteria decision analysis in environmental sciences: Ten years of applications and trends. Science of the Total Environment, 409(19), pp. 3578-3594.

Huang, S. J. & Liu, X. Z., 2013. Application of artificial bee colony-based optimization for fault section estimation in power systems. International Journal of Electrical Power & Energy Systems, 44(1), pp. 210-218.

Hwang, C. L. & Yoon, K. P., 1995. Multiple Attribute Decision Making and Introduction. London: Sage Publication.

Hwang, C. L. & Yoon, K., 1981. Multiple Attribute Decision Making Methods and Applications. In: a state of the art survey. Springer-Verlag, p. 181.

Jones, D. & Tamiz, M., 2010. Practical Goal Programming. In: Volume 141 of International Series in Operations Research and Management Science Series. Springer.

Johnson, N. F., 2011. Simply Complexity: A Clear Guide to Complexity Theory. Oneworld Publications.

Kahneman, D., 2011. Thinking, Fast and Slow. Allen Lane.

Kahneman, D. & Tversky, A., 1979. Prospect Theory: An analysis of decision under risk. 47(2).

Karaboga, D., 2005. An idea based on Honey Bee Swarm for Numerical Optimization. Technical Report 06 Erciyes University, Turkey.

Karaboga, N., 2009. A new design method based on artificial bee colony algorithm for digital IIR filters. Journal of the Franklin Institute, 346, pp. 328-348.

Keeney, R. L., 1992. Value-Focused Thinking: A Path to Creative Decision Making. Cambridge, Massachusetts: Harvard University Press.

Keeney, R. L. & Raïffa, H., 1976. Decisions with multiple objectives: preferences and value tradeoffs. New York: Wiley.

Keeney, R. L. & Gregory, R. S., 2005. Selecting Attributes to Measure the Achievement of Objectives. Operations Research, 53(1), pp. 1-11.

Keller, H. R. & Massart, D. L., 1991. Multicriteria decision making: A case study. Chemometrics and Intelligent Laboratory Systems, 11(2), p. 175–189.

Kennedy, J. & Eberhart, R., 1995. Particle Swarm Optimization. Proceedings of IEEE International Conference on Neural Networks IV, pp. 1942-1948.

Kennedy, J., Eberhart, R. & Shi, Y., 2001. Swarm Intelligence: The Morgan Kaufmann Series in Evolutionary Computation. Morgan Kaufmann.

Kirkpatrick, S., Gelatt, C. D. & Vecchi, M. P., 1983. Optimization by Simulated Annealing. Science, 220(4598), pp. 671-680.

Kjærulff, U. B. & Madsen, A. L., 2008. Bayesian Networks and Influence Diagrams: A Guide to Construction and Analysis. New York: Springer Science+Business Media.

Kletz, T. A., 2006. Hazop and Hazan. 4th Edition ed. IChemE.

Klopffer, W., 1997. Life Cycle Assessment: From the Beginning to the Current State. Environmental Science and Pollution Research, 4(4), pp. 223-228.

Koehn, D., 1997. Business and game-playing: The false analogy. Journal of Business Ethics, 16, pp. 1447-1452.

Lassiter, D. et al., 2009. The deliberation without attention effect: evidence for an artifactual interpretation. Psychological Science, 20(6), pp. 671-675.

Leng, R. B., Emonds, M. V. M., Hamilton, C. T. & Ringer, J. W., 2012. Holistic Route Selection. Organic Process Research and Development, 16(3), pp. 415-424.

Lidwell, W., Butler, J. & Holden, K., 2010. Universal Principles of Design. 2nd ed. Rockport Publishers.

Linkov, I. et al., 2006. From comparative risk assessment to multi-criteria decision analysis and adaptive management: Recent developments and applications. Environment International, 32, pp. 1072-1093.

Lootsma, F. A., 1999. MCDA in the Hands of Its Masters. In: Multi-Criteria Decision Analysis via Ratio and Difference Judgement. Springer US, pp. 259-270.

M. Tamiz , M., Mirrazavi, S. K. & Jones, D. F., 1999. Extensions of Pareto efficiency analysis to integer goal programming. Omega, 27(2), pp. 179-188.

Machina, M. J., 2008. non-expected utility theory. In: S. N. Durlauf & L. E. Blume, eds. The New Palgrave Dictionary of Economics, Second Edition. Palgrave Macmillan.

Manipura, A., 2012. Personal correspondence regarding "Chemical Product Engineering" on 5th May 2012

Malczewski, J., 1999. GIS and Multi-Criteria Decision Analysis. New York: John Wiley & Sons Inc.

Mareschal, B. & Brans, J. P., 1988. Geometrical representations for MCDA. the GAIA module.. European Journal of Operational Research, 34, pp. 69-77.

Mareschal, B. & Brans, J. P., 1992. PROMETHEE V: MCDM problems with segmentation constraints. ULB Institutional Repository 2013/9341, Universite Libre de Bruxelles.

Marks, R., 2004. Strategic Game Theory for Managers: Lecture 5-1. Sydney, The University of New South Wales.

Maystre, L., Pictet, J. & Simos, J., 1994. Les M´ethodes Multicrit`eres ELECTRE. Presses Polytechniques et Universitaires Romandes, Lausanne.

McCarthy, I. P., Tsinopoulos, C., Allen, P. & Rose-Anderssen, C. 2006. New Product Development as a Complex Adaptive System of Decisions. The Journal of Product Innovation Management, 23, pp. 437–456.

McMillan, J., 1996. Games, Strategies, and Managers: How Managers Can Use Game Theory to Make Better Business Decisions. Oxford University Press.

Mehta, S. S., 2008. Commercializing Successful Biomedical Technologies: Basic Principles for the Development of Drugs, Diagnostics and Devices. 1st ed. Cambridge University Press.

Metropolis, N., 1987. The Beginning of the Monte Carlo Method. Los Alamos Science, 15(584), pp. 125-130.

Millet, I. & Wedley, W. C., 2003. Modelling Risk and Uncertainty with the Analytic Hierarchy Process. Journal of Multi-Criteria Decision Analysis, 11(2), pp. 97-107.

Moisiadis, F., 1999. Improving the Scales Used in AHP for QFD. Transactions From the Eleventh Symposium on. Quality Function Deployment, June 12-18.

Moscato, P., 1989. On Evolution, Search, Optimization, Genetic Algorithms and Martial Arts - Towards Memetic Algorithms. Caltech Concurrent Computation Program.

Neri, F. & Cotta, C., 2012. Memetic algorithms and memetic computing optimization: A literature review. Swarm and Evolutionary Computation, 2, pp. 1-14.

Ng, K. M., 2004. MOPSD: a framework linking business decision-making to product and process design. Computers and Chemical Engineering, 29, pp. 51-56.

Opricovic, S., 1998. Multicriteria Optimization of Civil Engineering Systems. Faculty of Pennsylvania.

Opricovic, S. & Tzeng, G. H., 2004. Compromise solution by MCDM methods: A comparative analysis of VIKOR and TOPSIS. European Journal of Operational Research, 156, pp. 445-455.

Pareto, V., 1906. Manuale di economica politica, societa editrice libraria. Milano, Italy

Partovi, F. Y., 2007. An analytical model of process choice in the chemical industry. International Journal of Production Economics, 105(1), pp. 213-227.

Pascal, B. & Fermat, P. d., 1654-1660. Personal Communication.

Pavan, M. & Todeschini, R., 2009. 1.19 Multicriteria Decision-Making Methods. In: S. D. Brown, L. A. Sarabia & J. Trygg, eds. Comprehensive chemometrics: chemical and biochemical data analysis. Elsevier, pp. 591-629.

Pearce, D., 1998. cost-benefit analysis and environmental policy. Oxford review of economic policy, 14(4), pp. 84-100.

Petalas, Y. G., Parsopoulos, K. E. & Vrahatis, M. N., 2007. Memetic particle swarm optimization. Annals of Operations Research, 156, pp. 99-127.

Pham, D. T. et al., 2006. The bees algorithm – A novel tool for complex optimisation problems. Proceedings of the 2nd International Virtual Conference on Production Machines and Systems, pp. 454-461.

PhRMA, 2007. Drug Discovery and Development: Understanding the R&D Process. Pharmaceutical Research and Manufacturers of America, pp. 1-14.

Pirdashti, M., Ghadi, A., Mohammadi, M. & Shojatalab, G., 2009. Multi-Criteria Decision-Making Selection Model with Application to Chemical Engineering Management Decisions. World Academy of Science, Engineering and Technology, (49), pp. 54-59.

Pohekar, S. & Ramachandran, M., 2004. Application of multi-criteria decision making to sustainable energy planning—A review. Renewable and Sustainable Energy Reviews, 8, pp. 365-381.

Poli, R., 2008. Analysis of the Publications on the Applications of Particle Swarm Optimisation. Journal of Artificial Evolution and Applications.

Reay, D. A., Ramshaw, C. & Harvey, A. P., 2008. Process intensification: engineering for efficiency, sustainability and flexibility. Butterworth-Heinemann.

Rechenberg, I., 1971. Evolutionsstrategie – Optimierung technischer Systeme nach Prinzipien der biologischen Evolution, PhD Thesis.

Ridder, K. d. et al., 2008. Multi-criteria decision making in Product-driven Process Synthesis. Computer Aided Chemical Engineering, 25, pp. 1021-1026.

Romero, C., 2004. A general structure of achievement function for a goal programming model. European Journal of Operational Research, 153, pp. 675-686.

Roy, B., 1968. Classement et choix en presence de points de vue multiples (la methode ELECTRE). La Revue d'Informatique et de Recherche Opérationelle, 8, pp. 57-75.

Roy, B., 1978. ELECTRE III: Un algorithme de classements fondé sur une représentation floue des préférences en présence de critéres multiples. Cahiers du Centre d’Etudes de Recherche Opérationnelle, 20, pp. 3-24.

Roy, B. & Bertier, P., 1973. La Methode ELECTRE II - Une Application au Media-Planning. OR '72, M.Ross, North-Holland Pub. Company, pp. 291-302.

Roy, B. & Hugonnard, J. C., 1982. Ranking of suburban line extension projects on the Paris metro system by a multicriteria method. Transportation Research, 16(4), pp. 301-312.

Roy, B. & Skalka, J., 1984. ELECTRE IS : Aspects m´ethodologiques et guide d'utilisation. Document du LAMSADE 30, Universit´e Paris Dauphine.

Roy, B. & Bouyssou, D., 1993. Aide Multicritère d'Aide a la Décision: Méthodes et Cas. Paris: Economica.

Rubens, M., 1980. Analyse et aggrégation des préférences: modélisation, ajustement et résumé de données relationelles. Revue Belge de Statistique, d'Informatique et de Recherche Operationelle, 20, pp. 36-67.

Saaty, T. L., 1972. An eigenvalue allocation model for prioritization and planning. Energy Management and Policy Center, University of Pennsylvania.

Saaty, T. L., 1980. The Analytic Hierarchy Process. McGraw Hill International.

Saaty, T. L., 1994. How to Make a Decision: The Analytic Hierarchy Process. Interfaces, 24(6), pp. 19-43.

Saaty, T. L., 1996. Decision Making with Dependence and Feedback: The Analytic Network Process. Pittsburgh, Pennsylvania.: RWS Publications.

Saaty, L. T. & Vargas, L. G., 2012. How to Make a Decision. In: Models, Methods, Concepts & Applications of the Analytic Hierarchy Process. Springer.

Saling, P. et al., 2002. Eco-efficiency Analysis by BASF: The Method. The International Journal of Life Cycle Assessment, 7(4), pp. 203-218.

Salo, A. A. & Hämäläinen, R. P., 1997. On the measurement of preferences in the analytic hierarchy process. Journal of Multi-Criteria Decision Analysis, 6(6), pp. 309-319.

Salminen, P., Hokkanen, J. & Lahdelma, R., 1998. Comparing multicriteria methods in the context of environmental problems. European Journal of Operational Research, 104(3), pp. 485-496.

Sayyadi, M. K. & Makui, A., 2012. A new view to uncertainty in Electre III method by introducing interval numbers. Decision Science Letters, 1, pp. 33-38.

Schrage, M., 2003. Daniel Kahneman: The Thought Leader Interview. Strategy and Business, (33).

Schwefel, H. P., 1974. Numerische Optimierung von Computer-Modellen, PhD Thesis.

Sethi, R. & Iqbal, Z., 2008. Stage-Gate Controls, Learning Failure, and Adverse Effect on Novel New Products. Journal of Marketing, 72(1), pp. 118-134.

Shah, N., 2005. Process industry supply chains: Advances and challenges. Computers and Chemical Engineering, 29, pp. 1225-1235.

Sharratt, P., 2011. Whole Process Design. In: I. Houson, ed. Process Understanding: For Scale-Up and Manufacture of Active Ingredients. Weinheim, Germany: WILEY-VCH Verlag, pp. 323-341.

Simon, H. A., 1992. What is an explanation of behaviour? Psychological Science, 3, pp. 150-161.

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

Smith, J. E. & Winterfeldt, D. V., 2004. Decision analysis in Management Science. Management Science, 50(5), pp. 561-574.

Stewart, T. J., 2005. Dealing with uncertainties in MCDA. In: J. Figueira, S. Greco & M. Ehrgott, eds. Multi-criteria decision analysis - State of the Art Annotated Surveys. New York: Springer.

Stoner, J. A. F., 1961. A comparison between individual and group decisions involving risk. Masters Thesis, M.I.T., School of Industrial Management.

Sugiyama, H., Fischer, U., Hungerbühler, K. & Hirao, M., 2008. Decision framework for chemical process design including different stages of environmental, health, and safety assessment. AIChE Journal, 54(4).

Suri, B. & Kalkal, S., 2011. Review of Artificial Bee Colony Algorithm to Software Testing. International Journal of Research and Reviews in Computer Science, 2(3), pp. 706-711.

Tamiz, M., Jones , D. F. & El-Darzi, E., 1995. A review of Goal Programming and its applications. Annals of Operations Research, 58(1), pp. 39-53.

Tamiz, M., Jones, D. & Romero, C., 1998. Goal programming for decision making: An overview of the current state-of-the-art. European Journal of Operational Research, 111, pp. 569-581.

Tamiz, M., Mirrazavi, S. K. & Jones, D. F., 1999. Extensions of Pareto efficiency analysis to integer goal programming. The International Journal of Management Science, 27, pp. 179-188.

Terashi, M. & Umeda, T., 1991. A Method for Value-System Design and Evaluation of Manufacturing Systems. Proceedings of PSE'91, Montebello, Canada, p. III.22.1.

Trepel, C., Fox, C. R. & Poldrack, R. A., 2005. Prospect theory on the brain? Toward a cognitive neuroscience of. Cognitive Brain Research, 23, pp. 34-50.

Triantaphyllou, E., 2000. Multi-Criteria Decision Making Methods: A Comparative Study. 1st ed. Springer.

Triki, E., Collette, Y. & Siarry, P., 2005. A theoretical study on the behaviour of simulated annealing leading to a new cooling schedule. European Journal of Operational Research, 166, pp. 77-92.

Turocy, T. L. & Stengel, B. v., 2001. Game Theory (LSE-CDAM-2001-09). London School of Economics Research Report.

Tzeng, G. H., Lin, C. W. & Opricovic, S., 2005. Multi-criteria analysis of alternative-fuel buses for public transportation. Energy Policy, 33, pp. 1373-1383.

UCL, 2012. Risk Modelling and Management. [Online] Available at: http://www.ucl.ac.uk/syseng/research/risk-modelling-and-management [Accessed 10 09 2012].

US EPA, 2000. Guidelines for Preparing Economic Analyses. Washington: Environmental Protection Agency.

Van Der Pas, J. W. G. M. et al., 2010. Exploratory MCDA for Handling Deep Uncertainties: The Case of Intelligent Speed Adaptation Implementation. Journal of Multi-Criteria Decision Analysis, 17(1-2), pp. 1-23.

Venkatasubramanian, V., Rengaswamy, R., Yin, K. & Kavuri, S. N., 2003. A review of process fault detection and diagnosis Part I: Quantitative model-based methods. Computers and Chemical Engineering, 27, pp. 293-311.

Vohs, K. D. et al., 2005. Decision Fatigue Exhausts Self-Regulatory Resources - But So Does Accommodating to Unchosen Alternatives. The University of Chicago.

Von Neumann, J. & Morgenstern, O., 1947. Theory of games and economic behaviour. Princeton, N.J: Princeton University Press.

Wallenius, J. et al., 2008. Multiple Criteria Decision Making, Multiattribute Utility Theory: Recent Accomplishments and What Lies Ahead. Management Science, 54(7), pp. 1336-1349.

Watson, H. A., 1961. The Launch Control Safety Study. Murray Hill, NJ: Bell Labs.

Xiaoping, J., Zhang, T. & Shi, L., 2006. Multi-criteria Evaluation for the Chemical Industrial Parks. In: W. Marquardt & C. Pantelides, eds. 16th European Symposium on Computer Aided Process Engineering and 9th International Symposium on Process Systems Engineering. Elsevier, pp. 2177-2182.

Yu, W., 1992. ELECTRE TRI: Aspects methodologiques et manuel d'utilisation. Document du LAMSADE No. 74, Universit´e Paris-Dauphine.

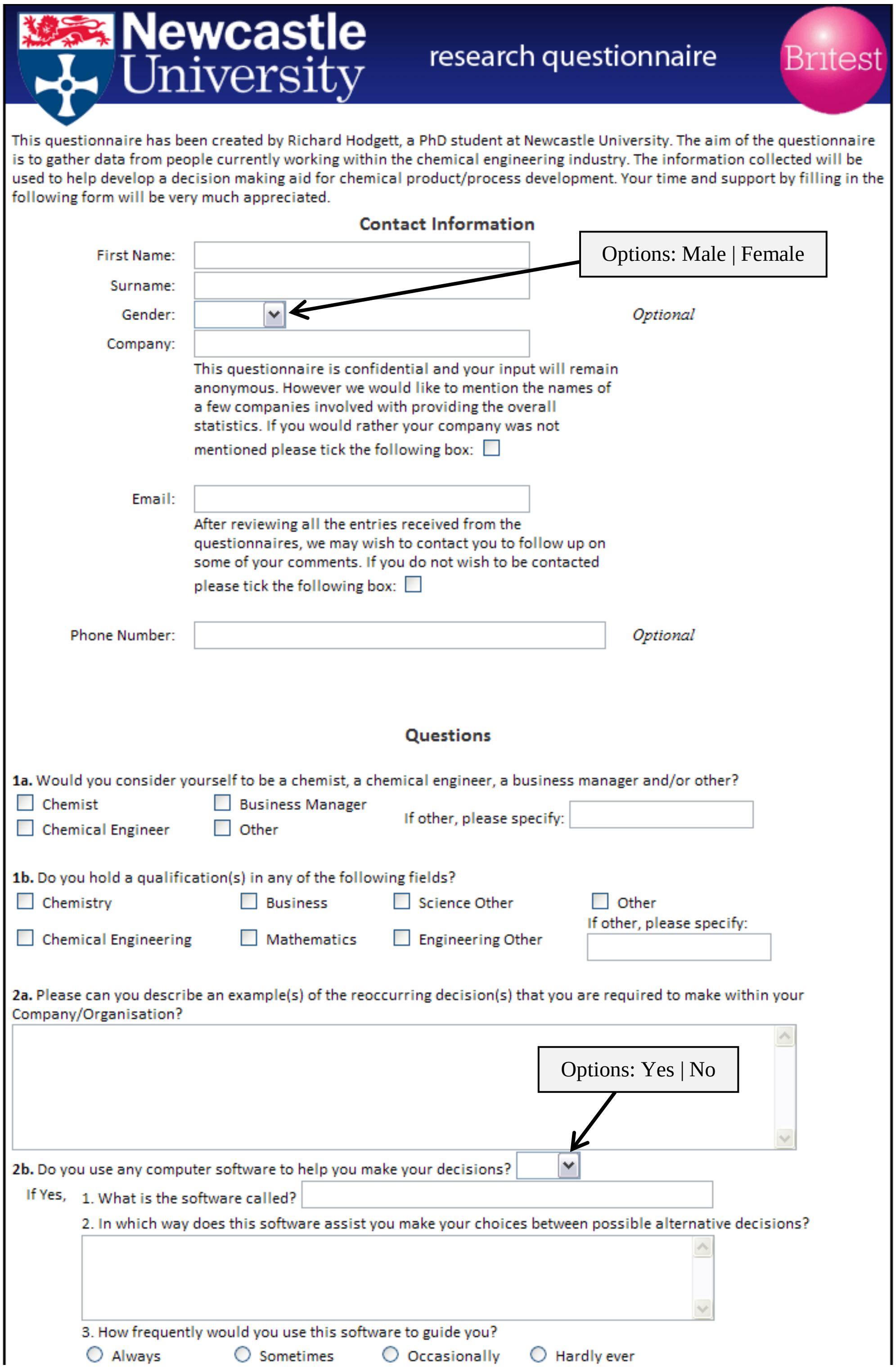
Zadeh, L., 1963. Optimality and Non-Scalar-Valued Performance. IEEE Trans Autom Control, 8(59-60).

Zadeh, L. A., 1965. Fuzzy Sets. Information and Control, 8(3), pp. 338-353.

Appendix A

This appendix contains the two structured questionnaires that are discussed in section 3.3. The options for the drop down boxes have been superimposed.

Questionnaire One (25/01/2010 – 19/02/2010)



Newcastle University

research questionnaire

Britest

This questionnaire has been created by Richard Hodgett, a PhD student at Newcastle University. The aim of the questionnaire is to gather data from people currently working within the chemical engineering industry. The information collected will be used to help develop a decision making aid for chemical product/process development. Your time and support by filling in the following form will be very much appreciated.

Contact Information

First Name:

Surname:

Gender: — Options: Male | Female — *Optional*

Company:

This questionnaire is confidential and your input will remain anonymous. However we would like to mention the names of a few companies involved with providing the overall statistics. If you would rather your company was not mentioned please tick the following box: ☐

Email:

After reviewing all the entries received from the questionnaires, we may wish to contact you to follow up on some of your comments. If you do not wish to be contacted please tick the following box: ☐

Phone Number: *Optional*

Questions

1a. Would you consider yourself to be a chemist, a chemical engineer, a business manager and/or other?

☐ Chemist ☐ Business Manager If other, please specify:

☐ Chemical Engineer ☐ Other

1b. Do you hold a qualification(s) in any of the following fields?

☐ Chemistry ☐ Business ☐ Science Other ☐ Other

If other, please specify:

☐ Chemical Engineering ☐ Mathematics ☐ Engineering Other

2a. Please can you describe an example(s) of the reoccurring decision(s) that you are required to make within your Company/Organisation?

Options: Yes | No

2b. Do you use any computer software to help you make your decisions?

If Yes, 1. What is the software called?

2. In which way does this software assist you make your choices between possible alternative decisions?

3. How frequently would you use this software to guide you?

○ Always ○ Sometimes ○ Occasionally ○ Hardly ever

If No, 1. Do you ever weigh out alternatives using pen and paper?

Options: Yes | No

2. If yes, in what way do you write or formulate your writing? (please provide an example if possible)

3. Does the business you work for use any timeline or gate system to stop and analyze projects/products as they are being developed?

If Yes, please specify and explain how it operates:

Options: Yes | No

4. Do you believe a decision-making tool for use during product/process development would be useful to you or to others in your company?

Please explain your answer:

5. For a decision making aid which is specifically designed to help throughout product/process development, please rate the importance of the following features from 1-10 (*1 being extremely unimportant and 10 being extremely important*):

	1	2	3	4	5	6	7	8	9	10
Intuitive user interface										
Speed of operation/input										
Influence from past decision-making or knowledge										
Compatibility with different Operating Systems (i.e. Windows, Mac, Linux etc)										
Contain functionality for quick fine tuning of your selections (sensitivity)										
Provide support for group decision making										
Provide functionality in the interface for writing notes to explain decisions										

6. For a decision making aid, would you prefer...

Please explain your choice:

Options: a system that only guides the user in the right direction quickly | a system that produces precise results for decisions with a lengthy entry procedure

Options: 5minutes | 15minutes | 30minutes | 1 hour | under 24 hours | 2-3 days | under a week | unlimited time

7. How long would you want to spend roughly entering data and analysing a single decision problem?

8. Is there anything else you would like to comment on regarding the construction of a decision making aid for the chemical industry?

Submit

Questionnaire Two (08/08/2010 – 27/08/2010)

Newcastle University research questionnaire Britest

This questionnaire has been created by Richard Hodgett, a PhD student at Newcastle University. This is the second and final questionnaire to gather data from people currently making decisions within the chemical industry. This questionnaire is aimed at any professional who makes decisions, managerial or other, during chemical product development. The questionnaire will take about 10minutes to complete. You do not have to have completed the first questionnaire to take part. Any information or responses you can provide will be very much appreciated.

Contact Information

First Name:

Surname:

Gender: ☐ — Options: Male | Female

Company:

This questionnaire is confidential and your input will remain anonymous. However we would like to mention the names of a few companies involved with providing the overall statistics. If you would rather your company was not mentioned please tick the following box: ☐

Email:

After reviewing all the entries received from the questionnaires, we may wish to contact you to follow up on some of your comments. If you do not wish to be contacted please tick the following box: ☐

Phone Number: *Optional*

Please describe your profession:

Please describe the typical decisions you make in your profession:

Are the decisions you make usually influenced from Quantitative data only, Qualitative data only or a mixture?

○ Quantitative ○ Qualitative ○ Quantitative and Qualitative

Section One: Problem Structuring

1. Do most of the decision problems you undertake involve decision-makers who are present to provide input or do you have to consider other external people's views and input?

○ Everyone is present ○ External influences have to be considered

2. Do you usually brainstorm a decision problem as an individual or as a group?

○ Individual ○ Group

3. When brainstorming the attributes/criteria/objectives for your decision problem do you prefer to organise your thoughts in the form of a list or a mind map?

○ A list (e.g. SWOT Analysis, Pros, Cons & Uncertainties, Needs and Wants etc).

○ A Mind Map (e.g. sketched mind map or a collection of post it notes/paper).

○ Neither. I do not use a brainstorming technique but I believe it would be helpful.

○ Neither. I do not use a brainstorming technique and I believe it wouldn't help me.

4. Do you find it difficult to define your attributes/criteria/objectives? In respect to naming them so other people understand the meaning and/or quantifying them?

Bad example: selecting "Safety" as a criterion: what form of safety does this mean? and how to quantify this criterion?
Good Example: selecting "Chemical Toxicity" as a criterion and using the LD50 index as a quantitative measure.

- Yes. I find it hard to name and source quantitative/qualitative data to define my decision criteria.
- I find it hard to name my decision criterion but not difficult to find data source(s).
- I find it easy to name my decision criterion but find it difficult to discover data source(s).
- No. I find it easy to name and source data to define each of my decision criteria.
- I do not organise my decision problems like this.

5. Do you find it difficult to organise your attributes/criteria/objectives into groups and sub groups?

- Yes, I find it hard to organise my decision attributes/criteria/objectives.
- No, I find it easy to organise my decision attributes/criteria/objectives for analysis.
- I do not usually structure my decision problems like this on paper. *

* If So, How do you organise your problem?

6. Do you know what all of your potential solutions/alternatives are when trying to make a decision?

- Yes. I know all of my decision alternatives.
- No. However, I can choose a number of alternatives which would be suitable to select from.
- No. I don't know of any potential solutions.

Section Two: Method Selection

7. Would you prefer to analyse your decision problem cognitively (ranking each attribute/criterion/objective against each other) or to source quantitative/qualitative data sources for each attribute/criterion/objective to construct a criteria matrix?

Generally a criteria matrix would take longer to construct than comparisons however the data is more precise for decisions under minimal risk and uncertainty.

- Consider the simplified problem manually (cognitively).
- Build a Criteria Matrix of data sources.

8. Would you prefer the results of a decision-making aid to be in the form of:

- A Ranking (rank alternatives from 1 to x).
- Quantifiable results (a number associated with each alternative).

9. For a comparison system (between two criteria or alternatives) what form of scale would you prefer to select from?

- Small Scale (for example 1-5) of heavily defined values.
- Medium Scale (for example 1-9) for moderately defined values.
- Large Scale (for example 1-100) for minimally defined values.

10. Do you believe you could select an appropriate distribution shape to define the risk involved with a certain value or set of criteria values?

- Yes. I understand mathematical distributions and the meanings of the shapes in accordance to risk.
- Yes. Under much guidance.
- No. I would prefer not to model risk in this way.

If you have any comments or questions regarding the questionnaire:

Submit

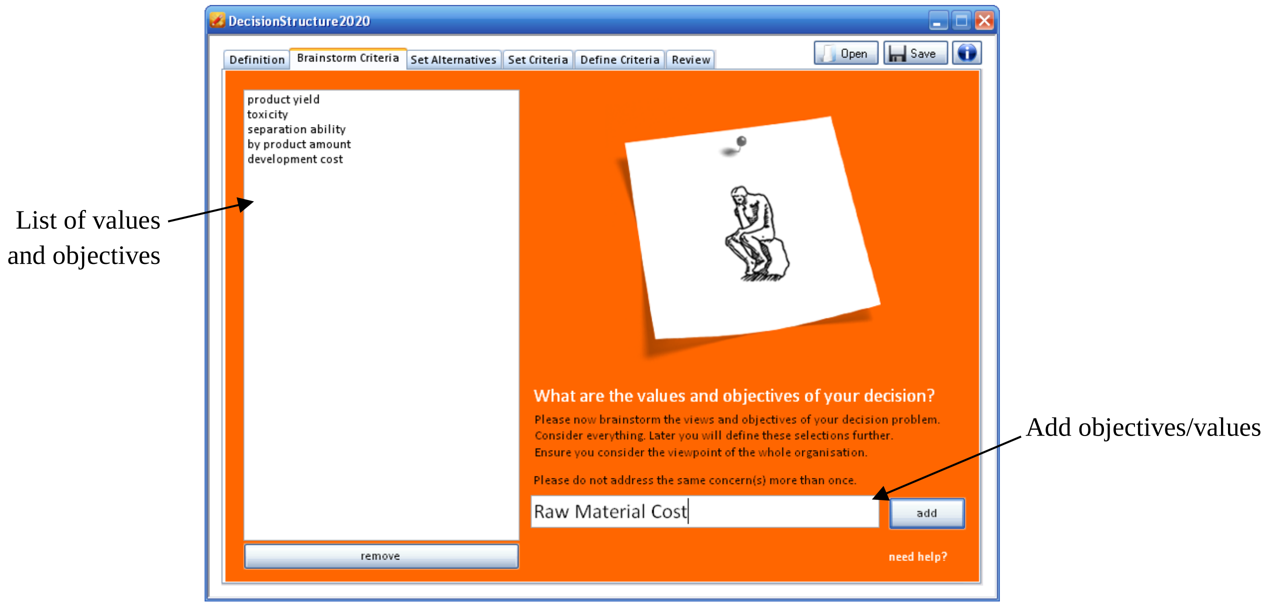
Appendix B

This appendix presents the Graphical User Interfaces (GUIs) of the ChemDecide framework. The GUIs must guide industrial users to structure their decision problem and evaluate three decision analysis methods. The analysis methods were developed with similar interfaces, utilising identical controls and forms where possible. As the industrial users may have little understanding of the decision-making processes, the GUIs need to be intuitive to lead the users through the process of building and evaluating a decision using each analysis tool. The GUIs of Decision Structure (the problem structuring tool) and the three analysis methods (AHP, MARE and RANK) are discussed independently followed by a section describing the contents of each decision file output.

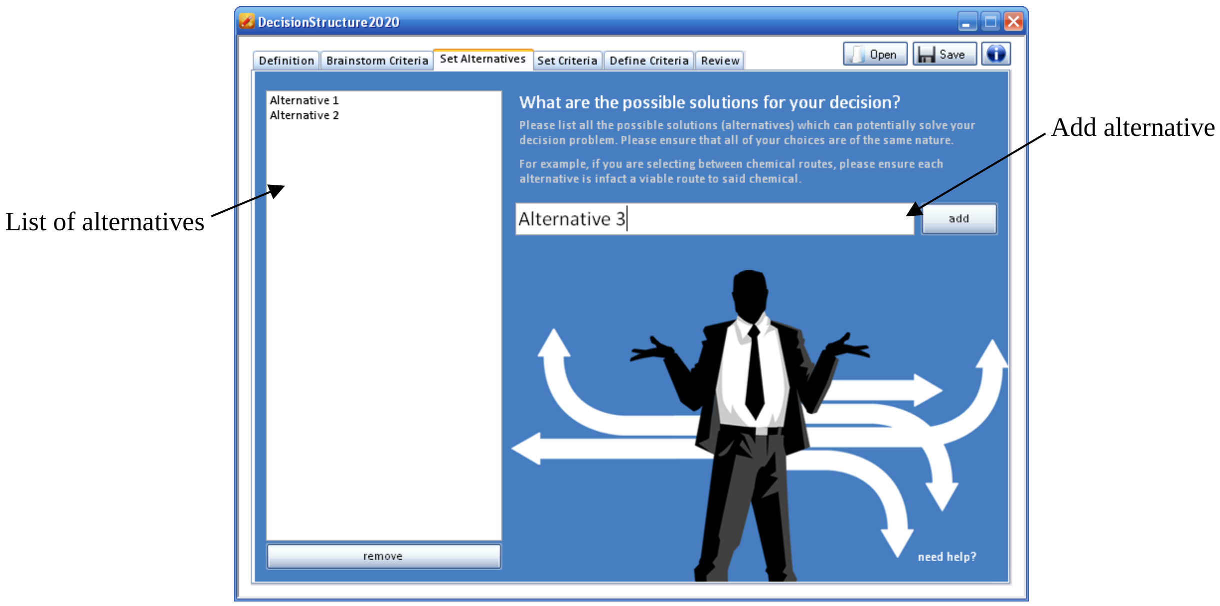
Decision Structure

After executing the decision structure program, a screen appears which allows the user to define their goal, team and decision timeframe:

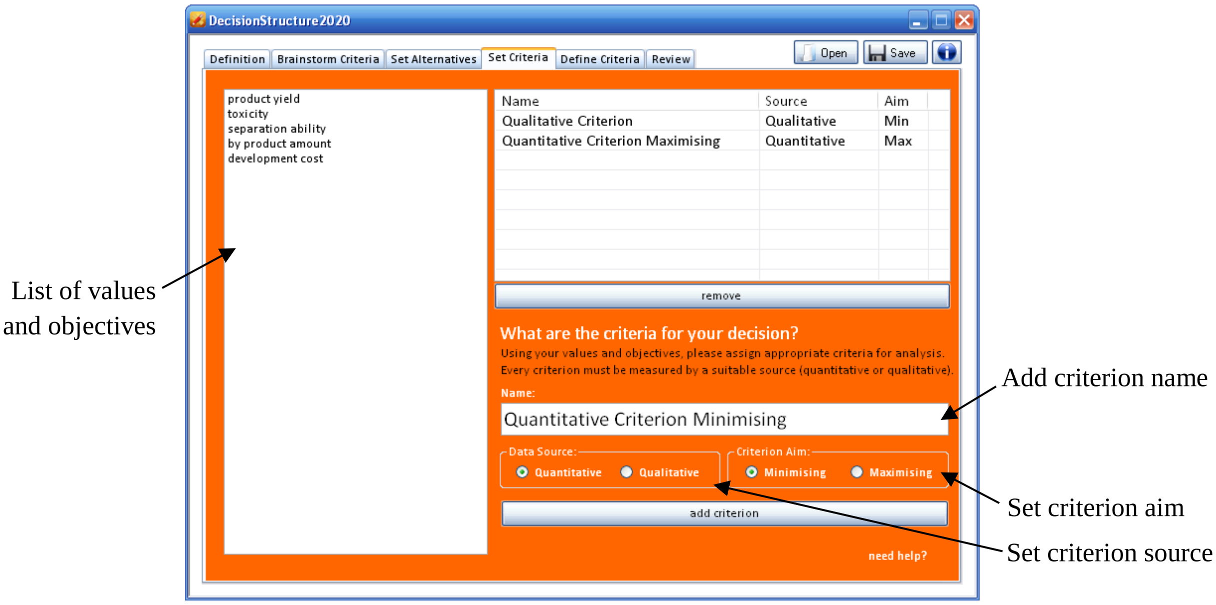
A tabular menu at the top allows progression through the various forms of the interface. The primary advantage of the tabular menu is that the user can return and advance to any section that needs adjustment. The second menu screen allows the user to brainstorm objectives and values. These will be used later to define appropriate criteria. The user can add and remove objectives/values from a list, there are no validation checks made on the information entered.

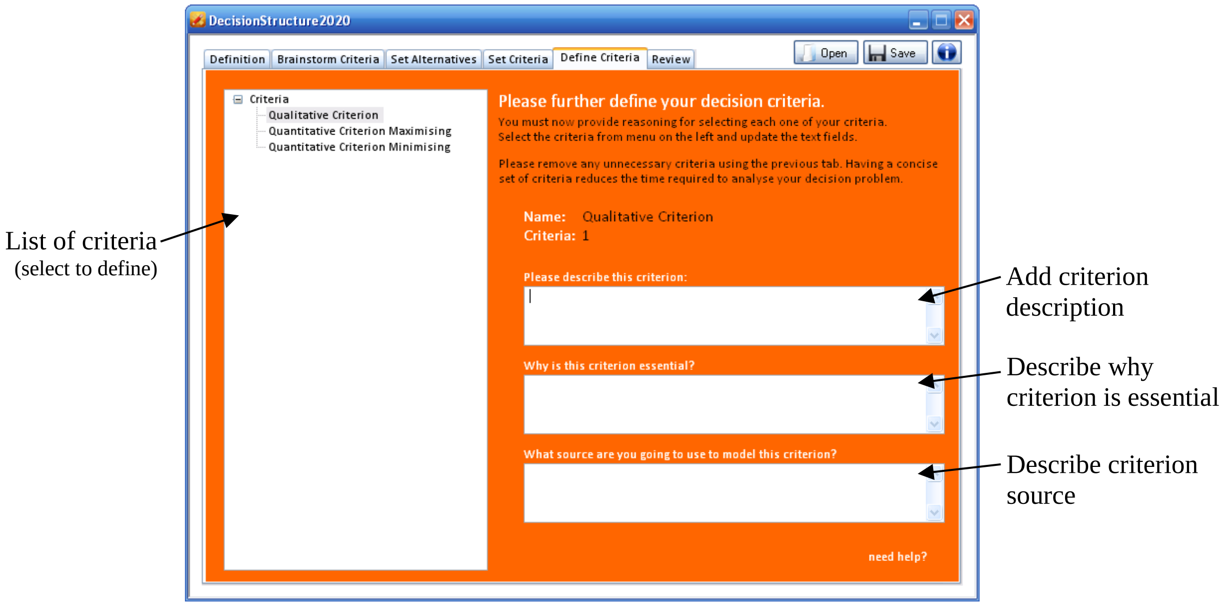


The third screen allows the user to define their decision alternatives. Similarly to the previous screen, the form permits the user to add and remove items from a list. As each alternative needs to be unique, a validation check is made when adding a new item to ensure there are no duplicates in the list.



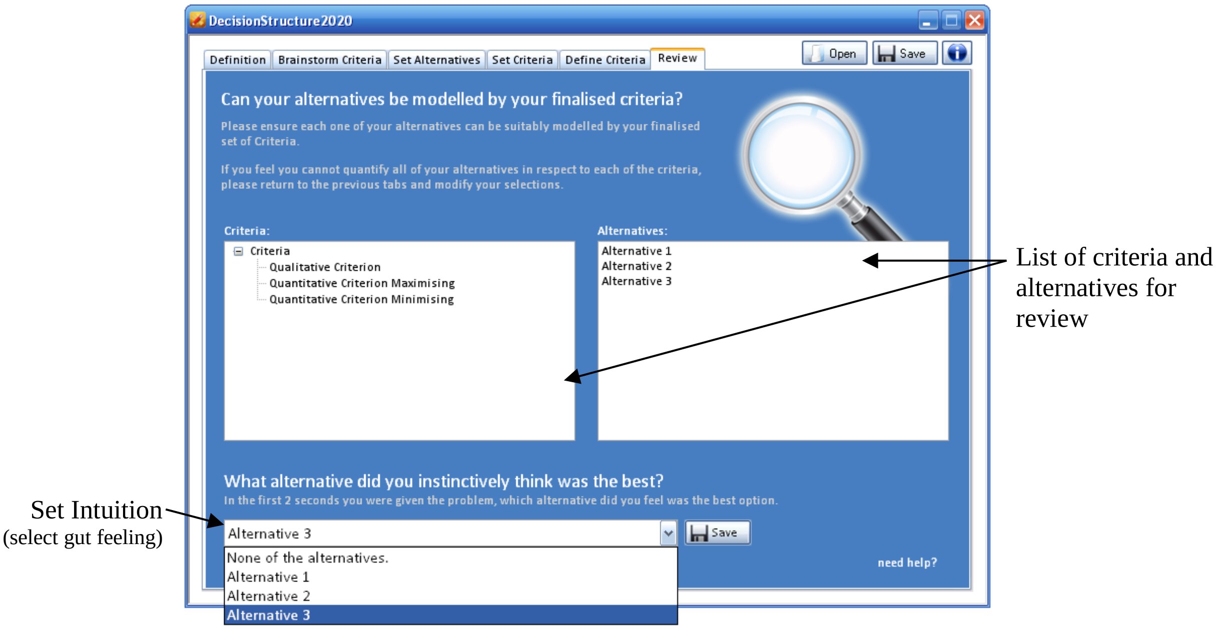
The next two screens require the user to define and explain their criteria. The previous list of values and objectives are shown to stimulate the user's thought process. Similarly to the alternative input, validation checks are made to ensure every criterion is unique.

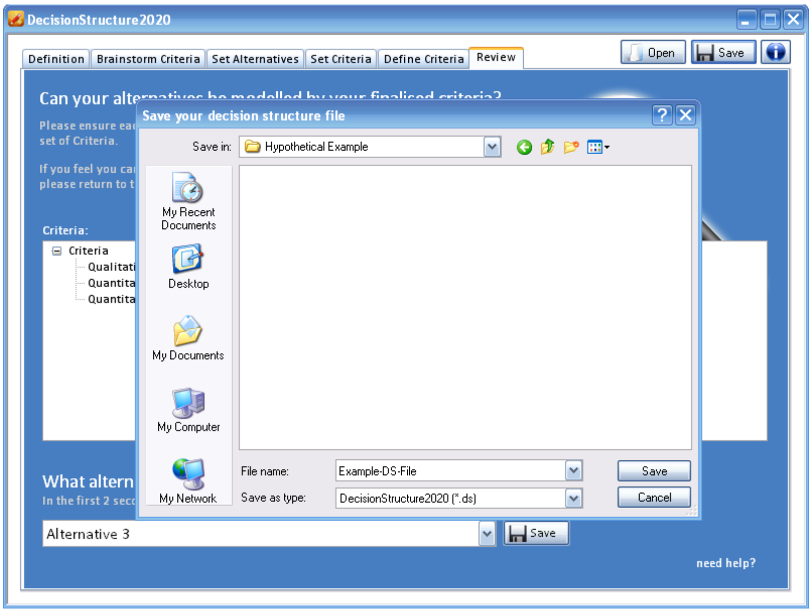




Once a set of criteria are established, the user must provide justification, a detailed description and a designated source for each criterion. This information is collected for the concluding analysis reports.

The final screen requires the user to validate their input by ensuring they have data for each alternative in respect to each criterion. The user can then select an alternative which they intuitively consider best and then save the decision file.

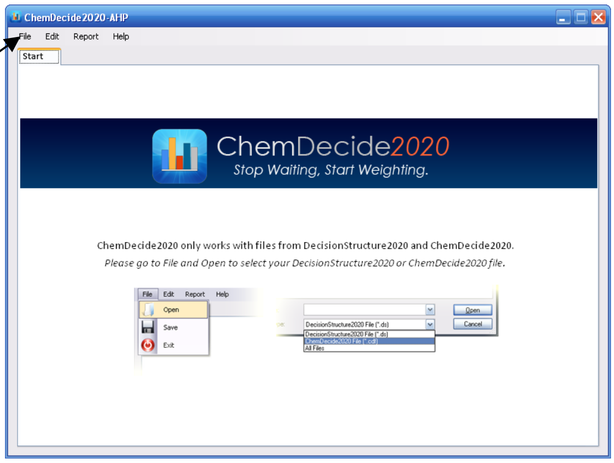




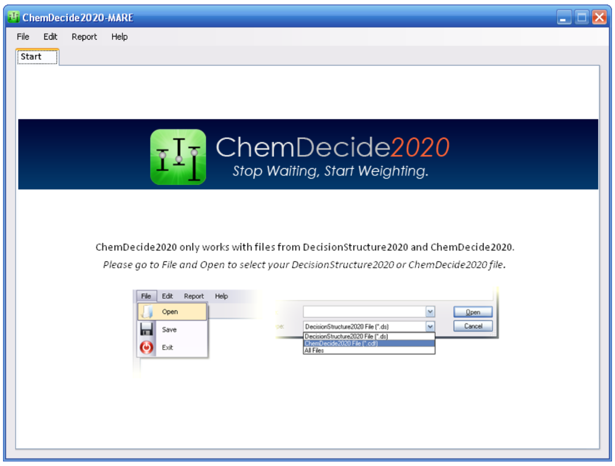
Analysis Tools

The initial screens of the analysis tools are shown below. The interfaces are identical besides individual icons which identify each method.

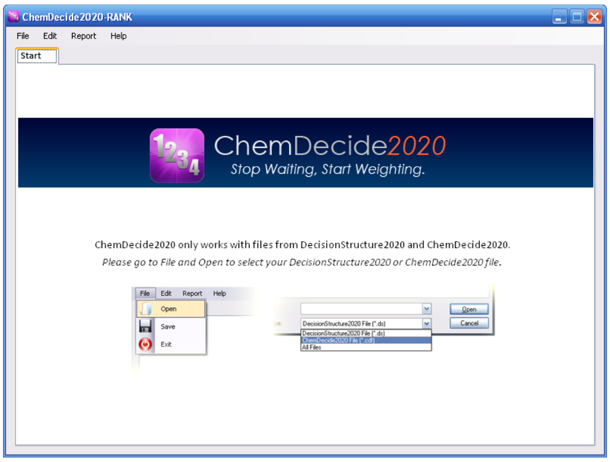
Selection Menu



AHP

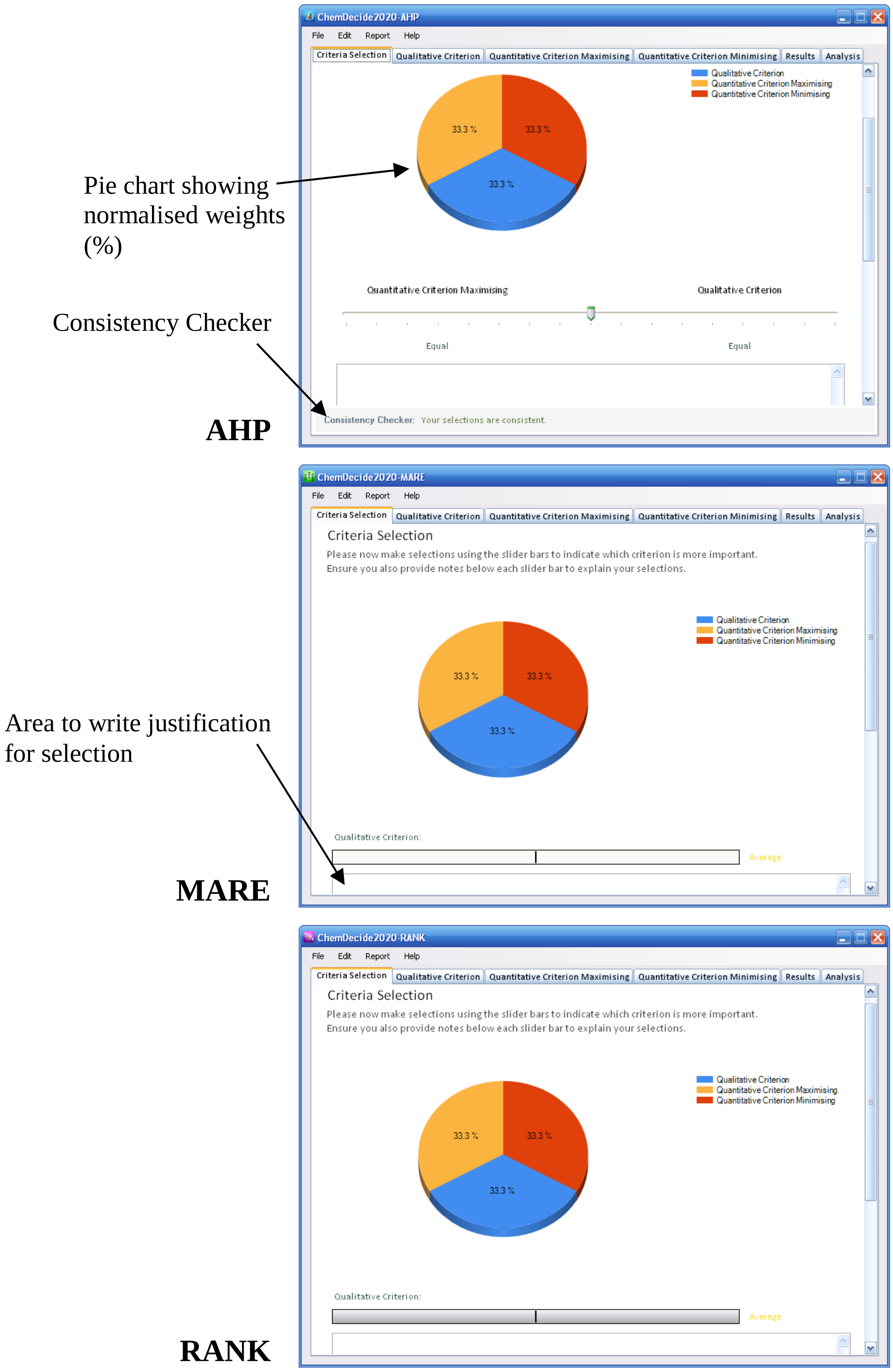


MARE



RANK

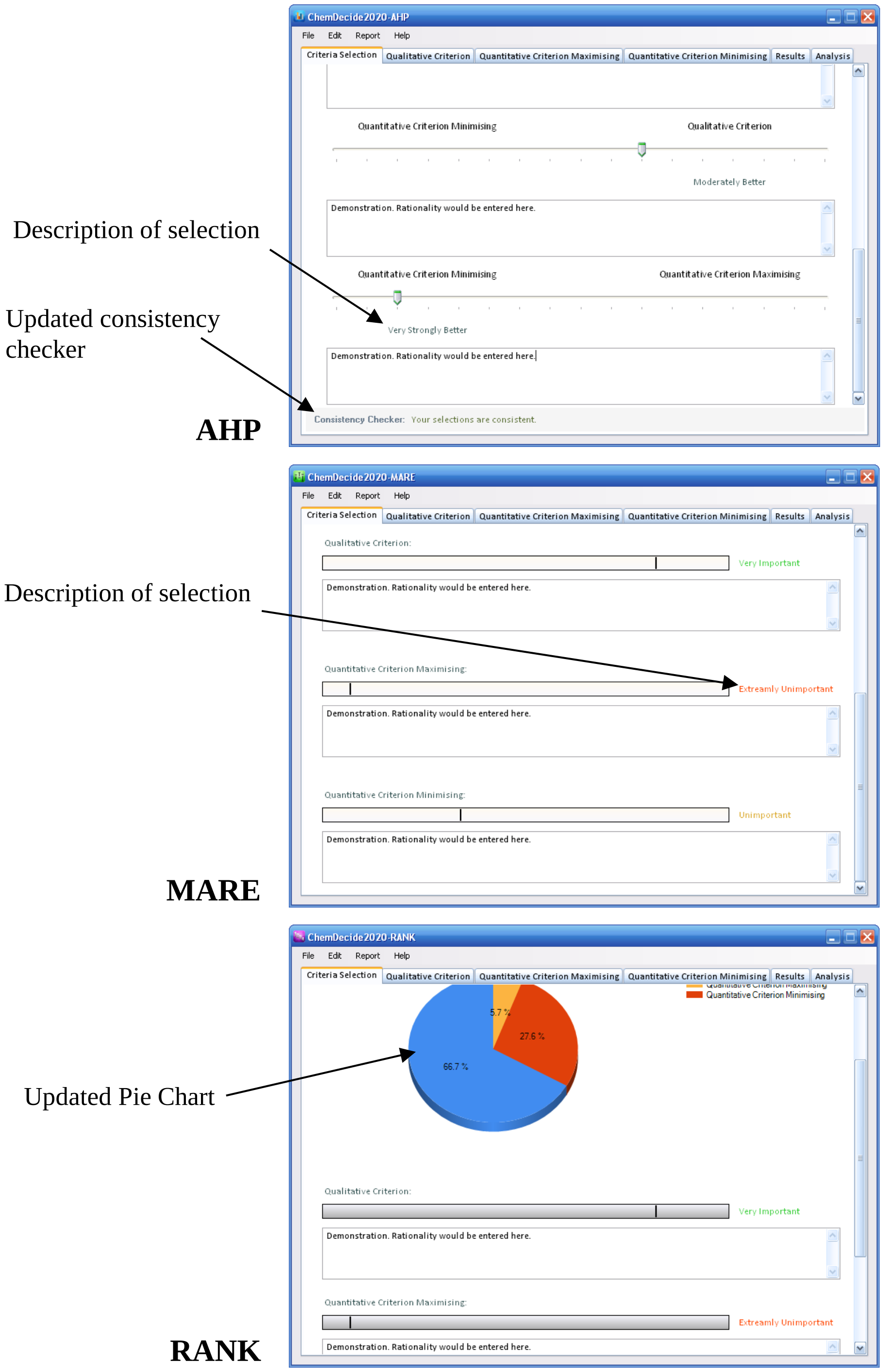
The user can load data from a Decision Structure file by accessing the selection menu at the top and selecting Open from the File menu. Once a file is opened, a tabular menu is generated with the first screen requiring the user to define their criteria weights using slider bars.



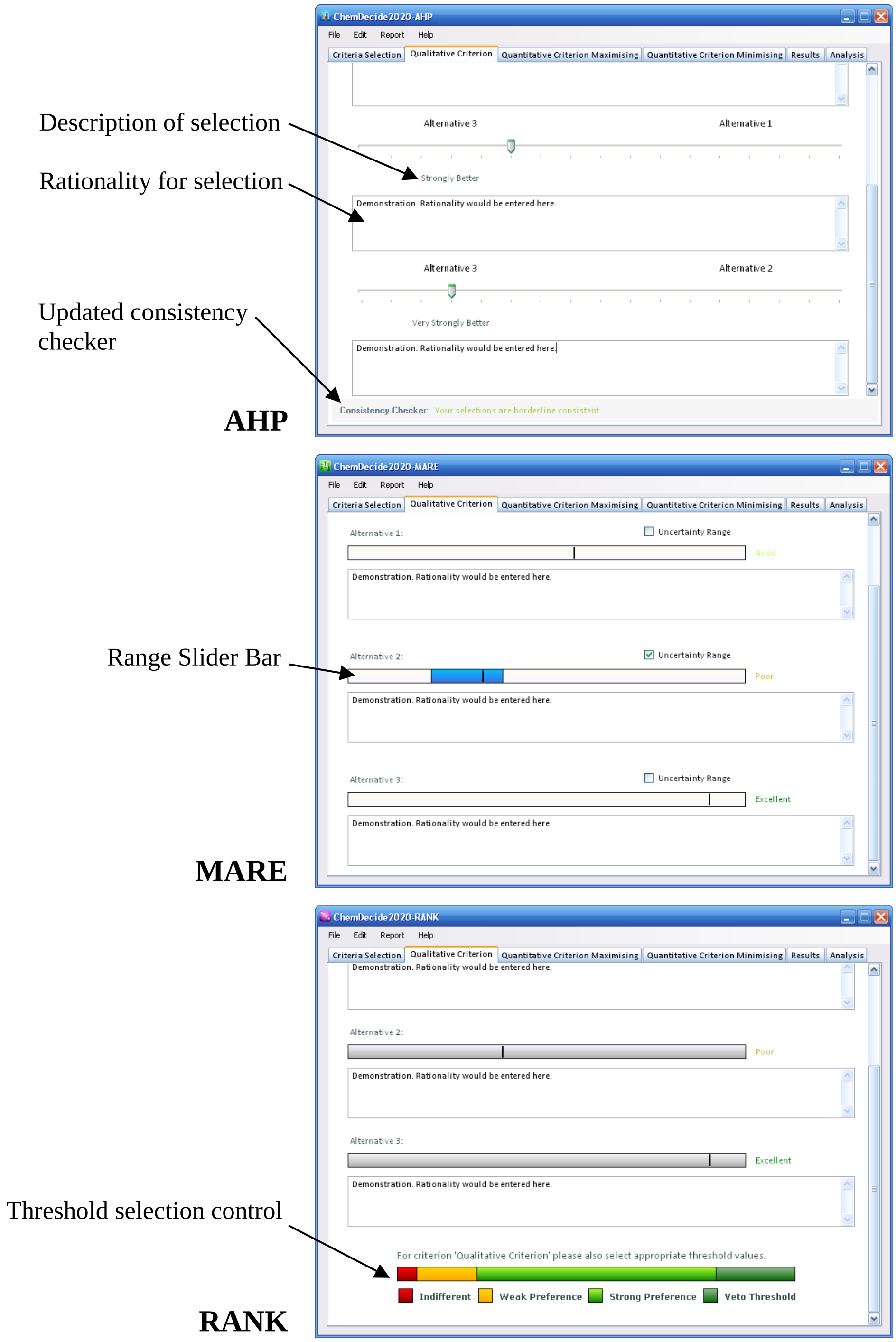
As the sliding bars are repositioned:

- The weights are calculated and displayed as normalised percentage values on a pie chart.

- A word model description of the selection is updated, for example: Average, Good, Very Good and Excellent.
- In AHP, the consistency checker is updated.



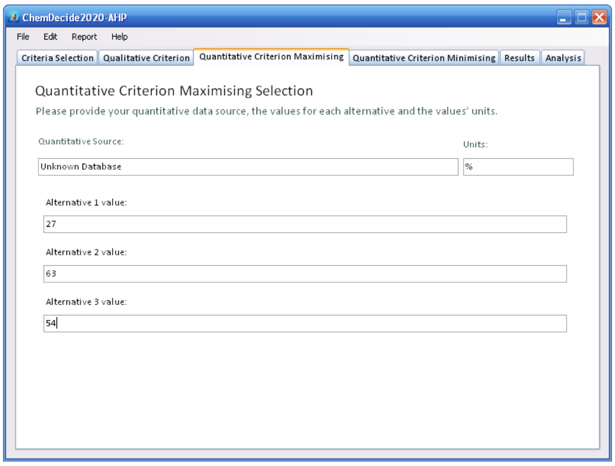
After the user is satisfied with their criteria weightings, they can progress through the tabular menu which contains a tab for each criterion. The screens for qualitative and quantitative criterion are different as they require different inputs. The qualitative data entry screens for each tool are shown below. In AHP, the user defines their pairwise comparisons using slider bars. A consistency checker is located at the bottom of the screen. As the slider bars are repositioned the Consistency Ratio (CR) is calculated and the status of the consistency check is updated.



In the MARE tool the user also defines each alternative with a slider bar but instead of using pairwise comparisons, the user positions the bar depending on preference with the far left being a low preference and the far right being a high preference. If the user is uncertain about a selection, they can enable the range slider bar by ticking the uncertainty range box. The range slider bar operates similarly to the previous slider bar but allows for the input of minimum, most likely and maximum values.

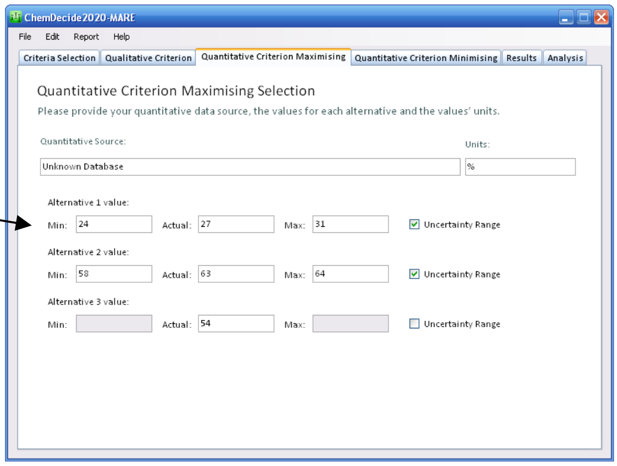
The RANK tool requires the user to define each alternative with a slider bar and select threshold values using the threshold selection control.

The quantitative data entry screens for each of the analysis tools are shown below.



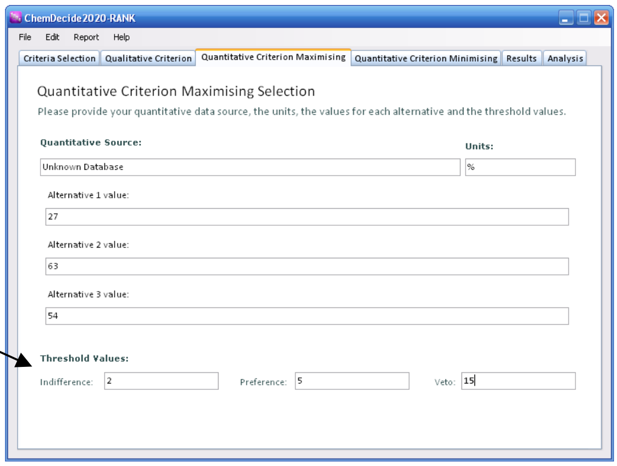
AHP

Uncertainty range selection



MARE

Threshold selections

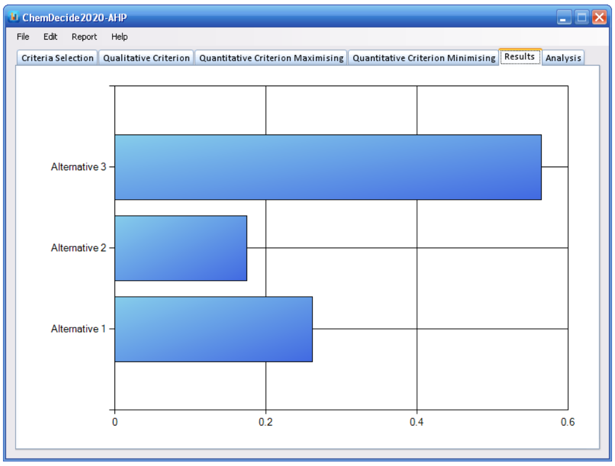


RANK

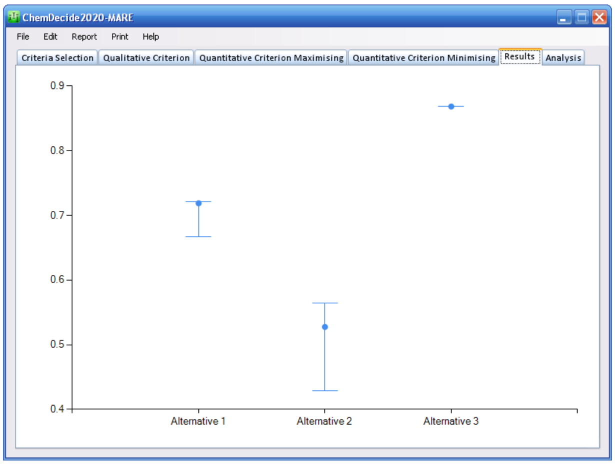
All three tools require the input of a source and measurement unit along with numerical scores for each alternative. The MARE method also allows the user to enter minimum and maximum values whilst the RANK method requires threshold values.

The final two screens in the tabular menu contain results and decision data:

AHP

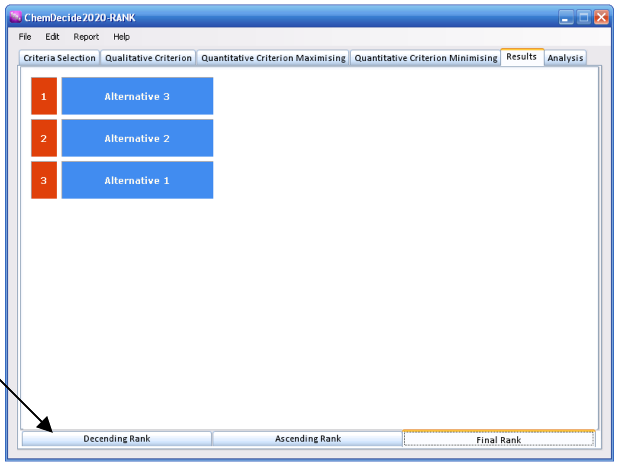


MARE

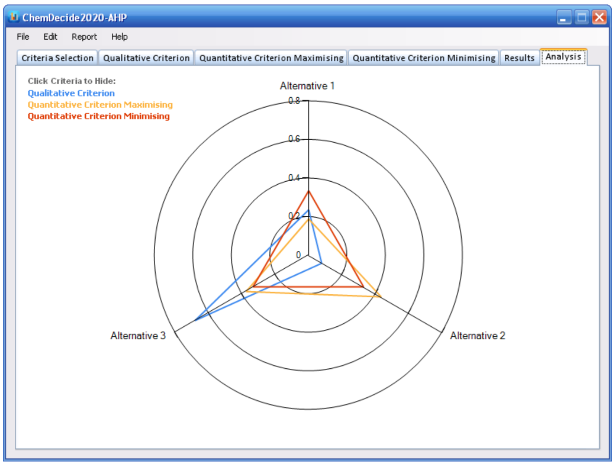


View different distillations

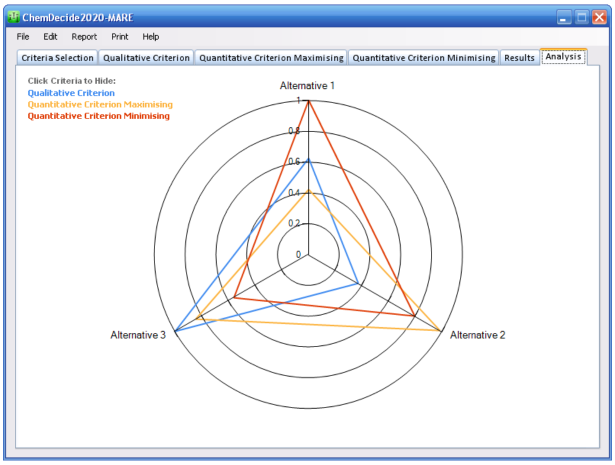
RANK



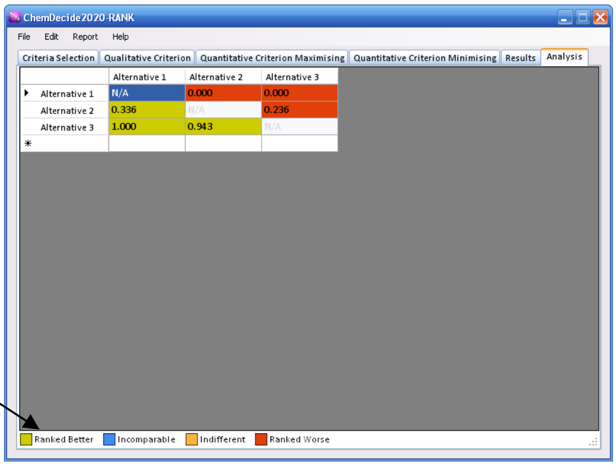
The results chart for AHP (shown above) provides numerical values in the form of a bar chart, MARE presents the minimum, most likely and maximum values for each alternative and RANK presents three rankings, descending, ascending and final.
The analysis charts for AHP and MARE show a spider diagram of the decision variables while the analysis chart for RANK shows the credibility matrix:



AHP



MARE



Key which updates when
particular values are selected

RANK

Post analysis, the user can choose to save a decision file or generate a report (in Word or PDF format) from the selection menu.

Decision File Output

Each of the four modules provides an output as an independent decision file. The data stored in each file is shown below:

Decision File Outputs

	DecisionStructure	AHP	MARE	RANK
File extension	*.ds	*.cdf	*.cdfm	*.cdr
Data Stored	Number of criteria, Number of alternatives, Goal, Decision-Makers, Alternative names, Criteria names/aim/source, criteria definitions, gut instinct selection.	All data in *.ds with: SliderBar values with rationality for criteria weights. SliderBar values with rationality for qualitative criteria. Data source, units and alternative values for quantitative criteria.	All data in *.ds with: SliderBar values with rationality for criteria weights. SliderBar and RangeSliderBar values with rationality for qualitative criteria. Data source, units and alternative values (min, likely and max) for quantitative criteria.	All data in *.ds with: SliderBar values with rationality for criteria weights. SliderBar and Threshold Selection Control values with rationality for qualitative criteria. Data source, units, alternative and threshold values for quantitative criteria.

Each algorithm stores every data element on a separate line within each decision file. Currently the data is not encrypted but the code was written such that an encryption algorithm could be implemented to secure the data. This will be necessary if companies wish to keep their decision-making information secure.

Appendix C

This appendix contains the decision data for the four analyses presented in Chapter 5.

Route Selection Problem (Robinson Brothers)

Interview transcript

The following information allowed the criteria weights and decision variables to be generated for this case study:

Route one:
"We would guess the overall non-isolated yield from this route to be ~80%. There are no toxic reagents and it would have been comfortably within the price target. The problem with this route is the isolation of the final product, which is highly water-soluble, and getting it away from the inorganic by-products would be a major problem. The chemistry involved was well known and would not have taken significant development time. Handling highly odorous material would be a major problem (show-stopper?) for many chemical manufacturers but high odour containment is a speciality for Robinson Brothers (RBL)."

Route two:
"We would have guessed an overall yield of ~70% from this route non-isolated. Separation of the final product from inorganics would be far less of a problem and we have carried out the chemistry on an analogue so know it well. The problem with this route is that the high cost of the starting material put us out of the park on overall economics."

Route three:
"We would have postulated an overall yield of ~75% from this route with less problems associated with separations of the required product from the probable by-products. Use of highly odorous material would again be an issue but not for RBL. The chemistry is solid and we would fully expect it to be successful. Problem with this route is that the starting material is moderately expensive and highly toxic."

AHP Analysis (Robinson Brothers)

The criteria matrix below shows the pairwise comparisons for the criteria weights:

	$c1$	$c2$	$c3$	$c4$	$c5$
$c1$	1	3	2	6	9
$c2$	0.3333	1	0.5	8	7
$c3$	0.5	2	1	5	8
$c4$	0.1666	0.125	0.2	1	5
$c5$	0.1111	0.1429	0.125	0.2	1

The table below shows the decision variables for the quantitative criterion:

	Source	**Units**	**Route 1**	**Route 2**	**Route 3**
c1. Yield	Estimated Values	%	80	70	75

The matrices below show the pairwise comparisons for the decision variables in respect to each criterion:

c2. Toxicity

	*route*1	*route*2	*route*3
*route*1	1	4	8
*route*2	0.25	1	4
*route*3	0.125	0.25	1

c3. Cost

	*route*1	*route*2	*route*3
*route*1	1	8	6
*route*2	0.125	1	0.3333
*route*3	0.1667	3	1

c4. Ease of Separation

	*route*1	*route*2	*route*3
*route*1	1	0.1429	0.1429
*route*2	7	1	1
*route*3	7	1	1

c5. Odour Expulsion

	*route*1	*route*2	*route*3
*route*1	1	0.2	0.5
*route*2	5	1	6
*route*3	2	0.1667	1

MARE Analysis (Robinson Brothers)

The table below shows the weight for each criterion:

	Score (/100)
c1. Yield	84
c2. Toxicity	42
c3. Price	56
c4. Separation	12
c5. Odour	6

The table below shows the decision variables in respect to each criterion:

		a1	a2	a3
c1. Yield Estimated Value (%)	Minimum	78	68	73
	Likely	80	70	75
	Maximum	82	72	77
c2. Toxicity Score (/100)	Minimum	69	20	5
	Likely	71	22	07
	Maximum	73	25	9
c3. Price Score (/100)	Minimum	74	5	15
	Likely	76	07	17
	Maximum	78	9	19
c4. Separation Score (/100)	Minimum	10	92	92
	Likely	12	94	94
	Maximum	14	96	96
c5. Odour Score (/100)	Minimum	9	71	14
	Likely	11	73	16
	Maximum	13	75	18

RANK Analysis (Robinson Brothers)

The criteria weights for RANK are identical to the MARE analysis.

The table below shows the decision variables in respect to each criterion:

	Thresholds		a1	a2	a3
c1. Yield Estimated Value (%)	Indifference:	1	80	70	75
	Preference:	5			
	Veto:	10			
c2. Toxicity Score (/100)	Indifference:	5	71	22	07
	Preference:	20			
	Veto:	50			
c3. Price Score (/100)	Indifference:	5	76	07	17
	Preference:	15			
	Veto:	65			
c4. Separation Score (/100)	Indifference:	5	12	94	94
	Preference:	20			
	Veto:	90			
c5. Odour Score (/100)	Indifference:	5	11	73	16
	Preference:	20			
	Veto:	55			

Degassing Methodology Selection (GSK)

AHP Analysis (GSK)

The matrix below shows the pairwise comparisons for the criteria weights:

	$c1$	$c2$	$c3$	$c4$	$c5$
$c1$	1	4	0.1111	1	3
$c2$	0.25	1	0.1111	0.3333	1
$c3$	9	9	1	9	9
$c4$	1	3	0.1111	1	2
$c5$	0.3333	1	0.1111	0.5	1

The table below shows the decision variables for the quantitative criterion:

	c3. Technically Possible Selection
Source	Experience
Units	Yes=1 and No=0
a1	1
a2	1
a3	1
a4	1
a5	0

The matrices below show the pairwise comparisons for the decision variables in respect to each qualitative criterion:

c1. Minimises Hold Up

	$a1$	$a2$	$a3$	$a4$	$a5$
$a1$	1	0.25	3	4	0.5
$a2$	4	1	6	5	2
$a3$	0.3333	0.1666	1	1	0.5
$a4$	0.25	0.2	1	1	0.5
$a5$	2	0.5	2	2	1

c2. Simple to Build

	$a1$	$a2$	$a3$	$a4$	$a5$
$a1$	1	0.3333	3	3	0.3333
$a2$	3	1	6	6	2
$a3$	0.3333	0.1666	1	1	0.3333
$a4$	0.3333	0.1666	1	1	0.3333
$a5$	3	0.5	3	3	1

c4. Available Now

	$a1$	$a2$	$a3$	$a4$	$a5$
$a1$	1	5	2	2	5
$a2$	0.2	1	0.25	0.25	3
$a3$	0.5	4	1	0.5	4
$a4$	0.5	4	2	1	4
$a5$	0.2	0.3333	0.25	0.25	1

c5. Low Cost

	$a1$	$a2$	$a3$	$a4$	$a5$
$a1$	1	1	3	3	5
$a2$	1	1	1	1	1
$a3$	0.3333	1	1	1	1
$a4$	0.3333	1	1	1	1
$a5$	0.2	1	1	1	1

MARE Analysis (GSK)

The table below shows the scores provided for the criteria weights:

	Score (/100)
c1. Minimises Hold Up	71
c2. Simple to Build	26
c3. Technically Possible	96
c4. Available Now	61
c5. Low Cost	50

The table below shows the decision variables for each criterion:

		a1	a2	a3	a4	a5
c1. Minimises Hold Up Score (/100)	Minimum	49	56	25	6	45
	Likely	61	88	40	40	50
	Maximum	75	97	48	48	60
c2. Simple to Build Score (/100)	Minimum	58	58	29	29	4
	Likely	62	70	35	36	50
	Maximum	66	75	51	52	93
c3. Technically Possible No=0 / Yes=1	Minimum	1	1	1	1	0
	Likely	1	1	1	1	0
	Maximum	1	1	1	1	0
c4. Available Now Score (/100)	Minimum	87	25	74	74	0
	Likely	91	76	85	85	17
	Maximum	100	83	97	97	39
c5. Low Cost Score (/100)	Minimum	69	25	34	28	3
	Likely	80	80	50	50	50
	Maximum	91	91	59	59	75

RANK Analysis (GSK)

The table below shows the scores provided for the criteria weights:

	Score (/100)
c1. Minimises Hold Up	72
c2. Simple to Build	39
c3. Technically Possible	94
c4. Available Now	64
c5. Low Cost	36

The table below shows the decision variables in respect to each criterion:

	Thresholds		a1	a2	a3	a4	a5
c1. Minimises Hold Up Score (/100)	Indifference:	5	60	79	34	50	74
	Preference:	20					
	Veto:	80					
c2. Simple to Build Score (/100)	Indifference:	5	62	62	39	38	50
	Preference:	20					
	Veto:	80					
c3. Technically Possible No=0 / Yes=1	Indifference:	0.1	1	1	1	1	0
	Preference:	1					
	Veto:	0					
c4. Available Now Score (/100)	Indifference:	5	82	51	70	70	8
	Preference:	20					
	Veto:	80					
c5. Low Cost Score (/100)	Indifference:	5	67	50	45	45	50
	Preference:	20					
	Veto:	80					

Premix Equipment Selection (FFIC)

AHP Analysis (FFIC)

The criteria matrix below shows the pairwise comparisons for the criteria weights:

	$c1$	$c2$	$c3$	$c4$	$c5$	$c6$	$c7$	$c8$	$c9$	$c10$
$c1$	1	5	0.25	0.3333	0.25	0.5	5	3	2	8
$c2$	0.2	1	0.25	0.3333	0.25	0.5	4	2	2	7
$c3$	4	4	1	2	1	1	5	6	5	9
$c4$	3	3	0.5	1	0.5	3	5	5	4	8
$c5$	4	4	1	2	1	3	5	6	5	9
$c6$	2	2	1	0.3333	0.3333	1	4	5	2	6
$c7$	0.2	0.25	0.2	0.2	0.2	0.25	1	2	1	4
$c8$	0.3333	0.5	0.1667	0.2	0.1667	0.2	0.5	1	1	3
$c9$	0.5	0.5	0.2	0.25	0.2	0.5	1	1	1	4
$c10$	0.1250	0.1429	0.1111	0.125	0.1111	0.1667	0.25	0.3333	0.25	1

The table below shows the decision variables for the quantitative criterion:

	c1. Capital cost at 50	**c2. Capital cost at 100**
Source	Estimated Figures	Estimated Figures
Units	Capital Expenditure **(£ * 1000)**	Capital Expenditure **(£ * 1000)**
a1	400	500
a2	500	500
a3	375	750
a4	200	400

The matrices below show the pairwise comparisons for the decision variables in respect to each criterion:

c3. Ease of cleandown

	$a1$	$a2$	$a3$	$a4$
$a1$	1	3	3	2
$a2$	0.3333	1	1	1
$a3$	0.3333	1	1	1
$a4$	0.5	1	1	1

c4. Complexity of solids feeding required

	$a1$	$a2$	$a3$	$a4$
$a1$	1	1	0.25	0.25
$a2$	1	1	0.25	0.25
$a3$	4	4	1	1
$a4$	4	4	1	1

c5. Ease of operation

	$a1$	$a2$	$a3$	$a4$
$a1$	1	0.5	0.5	0.5
$a2$	2	1	0.5	0.5
$a3$	2	2	1	1
$a4$	2	2	1	1

c6. Mechanical reliability

	$a1$	$a2$	$a3$	$a4$
$a1$	1	1	1	0.5
$a2$	1	1	1	0.5
$a3$	1	1	1	0.5
$a4$	2	2	2	1

c7. Material losses

	$a1$	$a2$	$a3$	$a4$
$a1$	1	1	3	3
$a2$	1	1	3	3
$a3$	0.3333	0.3333	1	1
$a4$	0.3333	0.3333	1	1

c8. Ease of modelling at lab scale

	$a1$	$a2$	$a3$	$a4$
$a1$	1	6	6	3
$a2$	0.1666	1	1	0.25
$a3$	0.1666	1	1	0.25
$a4$	0.3333	4	4	1

c9. Quality of vendor support

	$a1$	$a2$	$a3$	$a4$
$a1$	1	2	1	1
$a2$	0.5	1	0.5	0.5
$a3$	1	2	1	0.5
$a4$	1	2	2	1

c10. Power requirements

	$a1$	$a2$	$a3$	$a4$
$a1$	1	3	4	3
$a2$	0.3333	1	2	1
$a3$	0.25	0.5	1	0.5
$a4$	0.3333	1	2	1

MARE Analysis (FFIC)

The table below shows the scores provided for the criteria weights:

	Score (/100)
c1. Capital cost at 50	88
c2. Capital cost at 100	71
c3. Ease of cleandown	74
c4. Complexity of solids feeding required	63
c5. Ease of operation	76
c6. Mechanical reliability	58
c7. Material losses	50
c8. Ease of modelling at lab scale	42
c9. Quality of vendor support	50
c10. Power requirements	22

The table below shows the decision variables in respect to each criterion:

		a1	a2	a3	a4
c1. Capital cost at 50 £ * 1000	Minimum	350	400	300	160
	Likely	400	500	375	200
	Maximum	500	600	450	350
c2. Capital cost at 100 £ * 1000	Minimum	450	400	500	300
	Likely	500	500	750	400
	Maximum	600	600	900	700
c3. Ease of cleandown Score (/100)	Minimum	80	66	26	33
	Likely	80	66	26	33
	Maximum	80	66	26	33
c4. Complexity of solids feeding required Score (/100)	Minimum	28	32	61	61
	Likely	28	32	61	61
	Maximum	28	32	61	61
c5. Ease of operation Score (/100)	Minimum	66	65	64	65
	Likely	66	75	64	65
	Maximum	66	80	64	65
c6. Mechanical reliability Score (/100)	Minimum	50	50	50	50
	Likely	50	50	50	50
	Maximum	50	50	50	50
c7. Material losses Score (/100)	Minimum	72	56	33	44
	Likely	72	56	33	44
	Maximum	72	56	33	44
c8. Ease of modelling at lab scale Score (/100)	Minimum	75	24	23	28
	Likely	75	24	23	28
	Maximum	75	24	23	28
c9. Quality of vendor support Score (/100)	Minimum	50	48	50	18
	Likely	50	48	50	18
	Maximum	50	48	50	18
c10. Power requirements Score (/100)	Minimum	57	56	38	46
	Likely	57	56	38	46
	Maximum	57	56	38	46

RANK Analysis (FFIC)

The table below shows the scores provided for the criteria weights:

	Score (/100)
c1. Capital cost at 50	88
c2. Capital cost at 100	77
c3. Ease of cleandown	74
c4. Complexity of solids feeding required	62
c5. Ease of operation	73
c6. Mechanical reliability	50
c7. Material losses	68
c8. Ease of modelling at lab scale	44
c9. Quality of vendor support	50
c10. Power requirements	14

The table below shows the decision variables in respect to each criterion:

	Thresholds		a1	a2	a3	a4
c1. Capital cost at 50 £ * 1000	Indifference:	50	400	500	375	200
	Preference:	100				
	Veto:	200				
c2. Capital cost at 100 £ * 1000	Indifference:	100	500	500	750	400
	Preference:	200				
	Veto:	300				
c3. Ease of cleandown Score (/100)	Indifference:	5	75	62	32	39
	Preference:	20				
	Veto:	80				
c4. Complexity of solids feeding required Score (/100)	Indifference:	5	29	35	62	63
	Preference:	20				
	Veto:	80				
c5. Ease of operation Score (/100)	Indifference:	5	70	76	70	69
	Preference:	20				
	Veto:	80				
c6. Mechanical reliability Score (/100)	Indifference:	5	50	50	50	50
	Preference:	20				
	Veto:	80				
c7. Material losses Score (/100)	Indifference:	5	81	65	35	45
	Preference:	20				
	Veto:	80				
c8. Ease of modelling at lab scale Score (/100)	Indifference:	5	73	19	20	31
	Preference:	20				
	Veto:	80				
c9. Quality of vendor support Score (/100)	Indifference:	5	50	50	50	14
	Preference:	20				
	Veto:	80				
c10. Power requirements Score (/100)	Indifference:	5	72	62	19	30
	Preference:	20				
	Veto:	80				