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A holistic approach towards incorporating and/or improving the green sustainability of chemical process plant systems

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Abstract

Truly holistically green sustainability has yet to be fully realised within chemical process industries, particularly in consideration of socio-political perspectives that extend beyond operational compliance and workplace safety. The proposed project endeavoured to address this gap by incorporating/enhancing holistically green and sustainable approaches in the design and operation of chemical process plants (CPPs), using progressively more intricate multi-criteria decision-making (MCDM) frameworks. The frameworks acted as the project's analytical backbone that aimed to balance environmental, economic, social, and technical dimensions more equitably and rigorously.

To validate the methodology frameworks, four representative small-scale, modular CPP case studies were selected. Each of the following case studies reflected diverse sustainability challenges and process configurations: (i) sustainable water desalination, with a focus on low-energy membrane and solar-assisted distillation systems; (ii) isopropanol (IPA) synthesis via isopropyl acetate hydrolysis, emphasising green reaction pathways; (iii) green ammonia production via electrochemical nitrogen fixation and renewable hydrogen; (iv) lignocellulosic bioethanol production that integrates waste biomass valorisation. Process simulation for the IPA and green ammonia cases was carried out via Aspen Plus v12, to ensure realistic thermodynamic modelling and energy integration.

The MCDM frameworks were tailored for each case, with respect to their unique sustainability(-based) criteria and sub-criteria. Fuzzy Analytical Hierarchy Process (FAHP) was employed to rank and prioritise sustainable water desalination pathways. An integrated "hybrid" FAHP-TOPSIS (Technique for Order of Preference by Similarity to Ideal Solution) framework was implemented for IPA and green ammonia. Due to its strategic importance and complexity, green ammonia was further assessed via FAHP-VIKOR with PROMETHEE-II (Preference Rank Organisation Method for Enrichment Evaluations), to provide more nuanced rankings with regard to trade-offs and stakeholder value conflicts.

As a core outcome, a final (and most optimised) methodology framework was developed that facilitated the systematic integration of process systems engineering (PSE) tools with FAHP-VIKOR & PROMETHEE-II. This integrative approach proved to be particularly valuable as a viable decision-support tool for early-stage design and policy evaluation, that balances quantitative process modelling with qualitative sustainability assessments. Comprehensive sensitivity analyses evaluated robustness of the Posteriori MCDM frameworks. The proposed MCDM frameworks exhibited overall high stability, particularly within the final and most optimised framework, which remained largely consistent under perturbations of input weights and ranking thresholds. However, certain instabilities were observed and attributable to

uncertainties within VIKOR for specific sub-criterion, such as precise total equipment costs, which were often derived/estimated from secondary sources. Moreover, despite the methodological advancements, the frameworks retained a notable reliance on literature-derived values, especially for life cycle cost analysis (LCCA) and social-LCA (life cycle assessment). This dependency was primarily due to practical constraints, project resources, and scope limitations. These constraints highlight areas for potential enhancement.

Future research should aim towards addressing these gaps by incorporating real-time (primary) data, refining cost estimation models, and expanding the methodological framework to accommodate dynamic stakeholder input. Furthermore, a more in-depth and case-specific exploration of socio-political variables should be undertaken to elevate the framework from a primary technical tool, to a comprehensive sustainability governance platform.

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Glossary

Elements/Compounds/Ions

Ar = Argon

Ca = Calcium

CH_4 = Methane

Cl^- = Chloride ions

CO = Carbon Monoxide

CO_2 = Carbon Dioxide

H_2 = Hydrogen

H_2O = Water

H_2O_2 = Hydrogen Peroxide

K = Potassium

Mg = Magnesium

N_2 = Nitrogen

Na^+ = Sodium ions

NH_3 = Ammonia

SO_4^{2-} = Sulphate ions

Acronyms

AH = Acetone Hydrogenation

AHP = Analytic Hierarchy Process

AI = Artificial Intelligence

ANN = Artificial Neutral Network

ASU = Air Separation Unit

BGEA = Biomass Gasification Electrolysis

BLEVE = Boiling Liquid Expanding Vapour Explosion

CAPEX = Capital Expenditure(s)

CCR = Correct Classification Rate

CE = Circular Economy

CI = Consistency Index

CPP = Chemical Process Plant

CR = Consistency Ratio

DEEP = Desalination Economic Evaluation Program

ELECTRE = Elimination & Choice Expressing the Reality

ERG = Emergency Response Guideline

FAHP = "Fuzzy" Analytic Hierarchy Process

FS = Food Security

GC = Green Chemistry

GC-MS = Gas Chromatography-Mass Spectroscopy

GHG = Greenhouse gas

GW = Global Warming

H-B = Haber-Bosch

HPEA = Hydropower Electrolysis

IAH = Propylene Indirect Hydration

IEA = International Energy Agency

IPA = Isopropanol

ISO = International Standards Organisation

L&M = Labour & Management

LCA = Life Cycle Assessment

LCCA = Life Cycle Cost Analysis

MADM = Multi-Attribute Decision Making

MEEPRC = Ministry of Ecology & Environment of the People's Republic of China

MCDM/A = Multi-Criteria Decision Making/Analysis

MODM = Multi-Objective Decision Making

MSW = Municipal Solid Waste

Non-c tox = Human non-carcinogenic toxicity

NPV = Net Profit Value

NTEA = Nuclear High Temperature Electrolysis

ONS = Office of National Statistics

OPEX = Operating Expenditure(s)

PEM = Polymer Electrolyte Membrane

PH = Direct Propylene Hydration

PPM = Parts Per Million

PROMETHEE = Preference Ranking Organisation Method for Enrichment Evaluations

PSE = Process Systems Engineering

PVEA = Solar Photovoltaic Electrolysis

RKS-BM = Redlich-Kwong-Soave Modification

SAW = Simple Additive Weighting

SB(s) = Social Benefit(s)

SDG = Sustainable Development Goal

SED = Socio-Economic Development

Terr tox = Terrestrial toxicity

TFN(s) = Triangular Fuzzy Number(s)

TOPSIS = Technique for Order of Preference by Similarity to Ideal Solution

UN = United Nations

VIKOR = VIseKriterijumska Optimizacija I Kompromisno Resenje

WAVE = Water Application Value Engine

WEEE = Waste Electrical and Electronic Equipment

WGEA = Wind turbine Electrolysis

WPD = Whole Process Design

Calculations & Units of measurement

$\varphi(a)$ = Net outranking flows (of alternatives/pathways)

dB = Decibels

d.p. = Decimal Places

e_j = Entropy value

g_j = Coefficient of Difference

KJ/mol = Kilojoules per mole

Kg/hr = Kilograms per hour

Kmol/hr = Kilomoles per hour

L = Litre

RMB = Chinese Yuan

s.f. = Significant Figures

USD ($) = US Dollars

W_c = Comprehensive subjective weight

W_i = Combination weight

W_o = Objective weight

W_r = Subjective criteria weight

W_s = Subjective sub-criteria weight

1. Introduction

Green sustainability is a concept that has been explored in various existing literature, and multi-criteria decision making/analysis (MCDM/A) has been implemented towards more green and/or sustainable practices, including and beyond CPPs. This project expands upon the current literature (chapter 2) and addresses its gaps, with the development and implementation of progressively more intricate methodology frameworks, that balances the aforementioned dimensions of (green) sustainability with more rigor and equitability. At the time of writing the first progression review, preliminary work had been relatively limited. A relatively basic placeholder case study on biomass was initially defined to validate the project's proposed methodology framework. Since then, four representative case studies (1-3=simulation-based, 4=experiment-based) have been chosen to validate the project's proposed implementation of MCDM frameworks (chapters 4-6, 8):

1. Sustainable water desalination; specifically, low-energy membrane and solar-assisted distillation systems
2. Green reaction pathways for isopropanol (IPA) synthesis via isopropyl acetate hydrolysis
3. Green ammonia (NH_3) production via electrochemical nitrogen fixation and renewable hydrogen
4. Lignocellulosic bioethanol production that integrates waste biomass valorisation

1.1 General aims & objectives

The project's main aims, in no particular order of significance:

1) **Incorporate and/or enhance holistically green sustainability—socially, economically, environmentally, and technically—approaches in the design and operation for relatively small-scale and modular chemical process plant (CPP) systems.**

2) **Demonstrate and validate the capabilities of MCDM/A frameworks, within the context of more holistically-balanced dimensions of green sustainability (especially social/socio-political, beyond conventional considerations to workplace safety) and whole process design (WPD) philosophy.**

To do this, a series of objectives had to be fulfilled:

1) **Design, develop, and implement a series of progressively more intricate, novel Posteriori MCDM frameworks, that were tailored towards the unique sustainability-based criteria and sub-criteria of each case.**

Fuzzy Analytical Hierarchy Process (FAHP) was employed to rank and prioritise sustainable water desalination pathways based on various criteria; energy demand, brine disposal/management, social acceptance, and water recovery rate. The IPA synthesis and green NH_3 cases were assessed via a hybridised FAHP-TOPSIS (Technique for Order of Preference by Similarity to Ideal Solution) framework. Because of its strategic significance and complexity to holistically green sustainability, the green NH_3 case study was further assessed via FAHP-VIseKriterijumska Optimizacija I Kompromisno Resenje (VIKOR) with PROMETHEE-II (Preference Rank Organisation Method for Enrichment Evaluations). The resultant rankings were more in-depth and nuanced, with considerations of potential trade-offs and stakeholder value conflicts relevant to green NH_3 production.

2) **Develop and implement a final, optimised methodology framework from the aforementioned MCDM frameworks.**

3) **Provide a highly adaptable, decision-support tool for early-stage design and policy evaluation, that ideally balanced quantitative process modelling with qualitative sustainability assessments.**

The final, optimised framework involved the systematic integration of process systems engineering (PSE) tools via Excel and SimaPro software, with FAHP-VIKOR & Preference Ranking Organisation Method for Enrichment Evaluations (PROMETHEE-II). Specifically, the integration of the following PSE tools: life cycle assessment (LCA), life cycle cost analysis (LCCA), and social life-cycle cost assessment (social-LCA). Instead of a semi-random selection of sustainability-related sub-criteria based solely on the literature review, the definition of sub-criteria was based upon key sustainability factors derived via SimaPro and literature findings. Chapter 8 elaborates on the design, implementation, and validation of this final, optimised methodology framework via the experimental validation case study (bioethanol production).

1.2 Project structure & timetable

The project thesis consists of nine chapters, in the following order:

1) Introduction

2) Literature review

3) Overall methodology

4) Sustainable Water Desalination in Oman

5) IPA Case Study in China

6) Ammonia Production Case Study

7) Implementation of progressively intricate, integrated MCDM frameworks

8) Experimental Validation Case Study

9) Discussion

A Gantt chart was developed to chart the progress of the report via successive progression reviews, over the course of approximately three-and-a-half years (Appendix A).

2. Literature review

To fulfil the aims and objectives outlined in section 1.1, it was paramount to firstly develop a thorough, up-to-date literature review of the most relevant topics in (green) sustainability: defining "green" and "sustainability", green chemistry (GC), MCDM/A frameworks, and chemical process plants (CPPs). Key sustainability-related GC topics, the most prevalent MCDM methodologies, and the key components of CPPs must be considered for truly holistically green sustainability in (and beyond) chemical process industry. The literature review intends to highlight the gaps of previous studies, so that they can be addressed via the proposed methodology frameworks.

A. Green chemistry & sustainability

A.1 Background

For several decades, if not the last couple of centuries, society has regarded the natural world as a resource that can be mostly exploited without much consideration on the consequences, particularly when economic growth was the main (or only) priority (Hopwood et al., 2005; De Marco et al., 2019). During the last century, surges of rapid economic growth took place, led by globalisation and rapid urbanisation (Tobiszewski et al., 2009; Khoshnevis Yazdi & Dariani, 2019), that has triggered a significant growth in the global population and living standards (Tobiszewski et al., 2009; De Marco et al., 2019). On the other hand, this also led to greater natural resource depletion and increased pollution (Tobiszewski et al., 2009; De Marco et al., 2019; Khoshnevis Yazdi & Dariani, 2019). Moreover, the consequences—social, economic, and environmental—will only worsen with time, if not potentially become irreversible, without significant interventions and changes (Halada & Yagi, 2001; Dahle, 2007; Rockström, 2009). According to NOAA (2021), 2020 saw the highest-recorded amount of atmospheric carbon dioxide (CO_2) at 412.5 parts per million (ppm), despite the pandemic-caused economic slowdown (Lindsey, 2021). Fossil-fuel combustion, agriculture, and irresponsible land-use are the main sources of global greenhouse gas (GHG) emissions, exacerbating anthropogenic climate change and its impacts (Rockström, 2009; Krane, 2017; Sheldon, 2018; IPCC, 2022).

Therefore, to preserve our natural resources and mitigate against climate change, society must transition into a more sustainable state with a holistic mindset (Sheldon, 2018), as certain aspects of sustainability can often be ignored in favour of others; e.g., environmental over social (Geissdoerfer et al., 2017; Kirchherr et al., 2017). The 2015 and 2030 Sustainable Development Goals (SDGs) and the 169 associated targets, established by United Nations (UN) member states, are notable examples of holistic approaches towards sustainable societies, in which each SDG (out of 17 total) focuses on a social, economic, or environmental aspect of sustainable development and governance (Morton et al., 2019; Walsh et al., 2020; Cohen et al., 2021; Sarkodie, 2022). For example, SDG-12 (Responsible Consumption and Production) might seem to be solely focused on the environment, but the implementation of SDG-12 and its associated targets, such as resource and waste management, would require socio-economic and political changes. The following sections in 'Green chemistry (GC) & Sustainability' cover key overarching topics in (green) sustainability and sustainable development: the timeline of GC and sustainability, its definitions, and key GC topic areas that can be linked to green sustainability (or vice versa). Said key GC topics are circular economies (CEs) and biomass (biofuels and pyrolysis of municipal solid waste, MSW). These topics are essential towards the understanding and development of holistically green and/or sustainable MCDM frameworks, and how they can be applied towards various CPPs.

A.2 Research questions

1) What is GC and sustainability? How has the concept changed over time, and why? How does GC define and link with "green" sustainability, as opposed to solely sustainability?

2) What key areas of GC have been explored in the literature? What are the limitations? How could GC be applied to the aims of the project?

3) What is CE? What are the limitations of CEs, and how can they be resolved and/or mitigated? How can the concepts of CE be applied to the project?

4) What is pyrolysis? What is the current state of research into MSW pyrolysis, and its limitations? What can be learned from MSW pyrolysis, that can be applied to CPPs in terms of (holistic) green sustainability?

A.3 GC & Sustainability

A.3.1 What is GC?

GC is a means towards incorporating greater sustainability and sustainable development, to reduce the negative impacts towards human health and the environment via safe, non-toxic reagents and solvents in chemistry (Beach et al., 2009; Tobiszewski et al., 2009; Kalidindi & Jagirdar, 2012; Lewandowski, 2014; Sheldon, 2018; De Marco et al., 2019). Moreover, GC involves the adoption of safer, more efficient—in terms of energy and yields—methods and technique, such as catalysis, and greater reliance on renewable resources (Tobiszewski et al., 2009; Kalidindi & Jagirdar, 2012; Lewandowski, 2014; Sheldon, 2018; De Marco et al., 2019). Every stage in analytical chemistry, from collecting sample(s) to syntheses and result evaluations, has the potential to impact the environment and its inhabitants (Woodhouse & Breyman, 2005; Tobiszewski et al., 2009; De Marco et al., 2019). Additionally, analytical methodologies can also have negative multi-dimensional impacts; for example, the measuring of chemical oxygen demand in water involves the use of hexavalent chromium, which is carcinogenic and environmentally hazardous (Miller et al., 2001). Therefore, it is paramount that GC addresses as many potential negative impacts as possible with safer, more efficient, and more sustainable alternatives.

However, as stated by Anastas & Warner (1998), waste prevention is/should be the highest priority in GC (Appendix B). This means that the non-use of chemical solvents and reagents, whenever possible/feasible, is preferred over finding alternatives, regardless of their safeness and/or environmental friendliness (Woodhouse & Breyman, 2005; Beach et al., 2009; Melchert et al., 2012; De Marco et al., 2019). Furthermore, while sustainability and GC are linked (Woodhouse & Breyman, 2005; Beach et al., 2009), they are not interchangeable; GC should not automatically be considered sustainable. GC may offer safer and/or more efficient alternatives to substances and/or methods, but these have no guarantee of sustainability (Sheldon, 2018).

A.3.2 What is sustainability?

Sustainability is a multi-dimensional, multi-disciplinary concept with hundreds of varied definitions, to the extent where many arguments have taken place among researchers in numerous fields (Hopwood et al., 2005; Dahle, 2007; Johnston et al., 2007; Geissdoerfer et al., 2017). The etymology of the word "sustainability" originates from the French *soutenir*, which means "to support/hold up" (Brown et al., 1987). On a fundamental level, sustainability refers to the depletion of natural resources (Kerk & Manuel, 2008), which shrinks the global ecosystem, as it is unable to regenerate itself (Brown et al., 1987; De Marco et al., 2019). However, it was in 1987, when the Brundtland Commission established an overall accepted, modernised definition of sustainability or specifically "sustainable development": the needs of future generations should not be compromised by the needs and development of whom live in the present (Dahle, 2007; Bartelmus, 2013; Barbier and Burgess, 2015; De Marco et al., 2019). This definition was created from an increasing awareness of the links between socio-economic and environmental global issues, that would be required to transition into sustainable societies (Hopwood et al., 2005; Kerk & Manuel, 2008). That said, it is also argued that Brundtland's definition might be too anthropocentric, i.e., approaching sustainability and sustainable development in terms of how it benefits humanity more than the natural world itself (Hopwood et al., 2005). As it becomes increasingly more important that the natural world is preserved, outside of solely anthropocentric reasons, "sustainability" and "sustainable development" must be refined with a more holistic mindset, in which all dimensions and scales are addressed appropriately (Mulvihill et al., 2011; Kalidindi et al., 2012; Barbier and Burgess, 2015; De Marco et al., 2019). A more holistic mindset to sustainability, for example, would be comparable to abiding by the Triple Bottom Line—the three sustainability pillars: social, economic, and environmental—but more balanced and integrated, with consideration to spatial and temporal dimensions (Bartelmus, 2013; Geissdoerfer et al., 2017).

Section A.3.3 elaborates on the timeline of sustainability and GC, in regard to how both concepts have changed and developed over the years since their inception. Additionally, Sections A.4-.5 cover some key concepts in GC—CEs and biomass, respectively—and how they are linked to (green) sustainability.

A.3.3 Timeline of GC & Sustainability

As a concept, sustainability has existed for over several decades, if not centuries, from as far back as the Greco-Roman period (Mebratu, 1998; Du Pisani, 2006; Spindler, 2013; De Marco et al., 2019). The development of concepts like agriculture led to the devaluation of the natural world (Du Pisani, 2006), and driving revolutions to address resource scarcities that are themselves driven by increasing resource demands (Mebratu, 1998). For example, during the Victorian era, the "First" Industrial Revolution led to the proliferation of coal as an energy source, which led to the advent of steam power, that resulted in significant societal upheaval. Such an upheaval was triggered by numerous factors: rapid urbanisation, the evolution of science and technology in leaps and bounds, and an overall improvement in global living standards (Mebratu, 1998; Groumpos, 2021). And although the fundamental concept of sustainability had existed for centuries, the depletion and degradation of Earth's natural resources continued without much consideration to the multi-dimensional consequences (Tobiszewski et al., 2009). A rapidly growing global population and revolutions had created a mindset, that the natural world was for humanity to use as they saw fit, especially when it comes to economic growth (Worster, 1993; Mebratu, 1998).

GC has made significant steps towards global-scale and multi-dimensional awareness, as well as applications to sustainability and sustainable development (Tobiszewski et al., 2009; Farias & Fávaro, 2011; De Marco et al., 2019). Appendix C illustrates the overall timeline of sustainability and GC. That said, greater progress towards sustainability can still be implemented; the main issues are balancing economic viability and GC technical capabilities with any social, political, and environmental concerns (De Marco et al., 2019), via a holistic mindset. For the project, this would involve the utilisation of individual and/or integrated Posteriori MCDM frameworks (Al-Majali & Zobaa, 2025), such as Fuzzy AHP (FAHP) or FAHP-VIKOR.

A.4 Circular economies (CEs)

A.4.1 CEs as a concept

Global sustainable development can be defined as the linear, throughput flow of energy and materials between the natural world and the economy (Korhonen et al., 2018). Moreover, it is the addressing of present needs/demands, without compromising the needs and opportunities of/for future generations (Barbier and Burgess, 2015). However, linear flow systems, also known as cradle-to-grave, are not truly sustainable; materials and products become "downcycled" (i.e. downgraded) upon recycling, which can be harmful to human health and the environment (Braungart et al., 2007). Specifically, linear flow systems cause the global ecosystem to shrink (Brown et al., 1987), and the deterioration of the system itself, both qualitatively and quantitatively from increasing resource demands (Brown et al., 1987; Mihelcic et al., 2003; Korhonen et al., 2018). Therefore, a cyclical flow of energy and materials needs to be implemented in its place, in the form of circular economies (CEs) (Ghisellini et al., 2016; Korhonen et al., 2018). The concept, as best exemplified by Mihelcic et al. (2013) in Figure 2.1, was introduced by Peace & Turner (1989), which in turn was influenced by the research of Boulding (1966), who described the planet as a closed system that requires economic-environmental equilibrium. If successfully implemented, CEs have the potential to address green sustainability and sustainable development in a multi-dimensional manner; socially, economically, politically, and environmentally (Ghisellini et al., 2016; Lieder & Rashid, 2016; Korhonen et al., 2018).

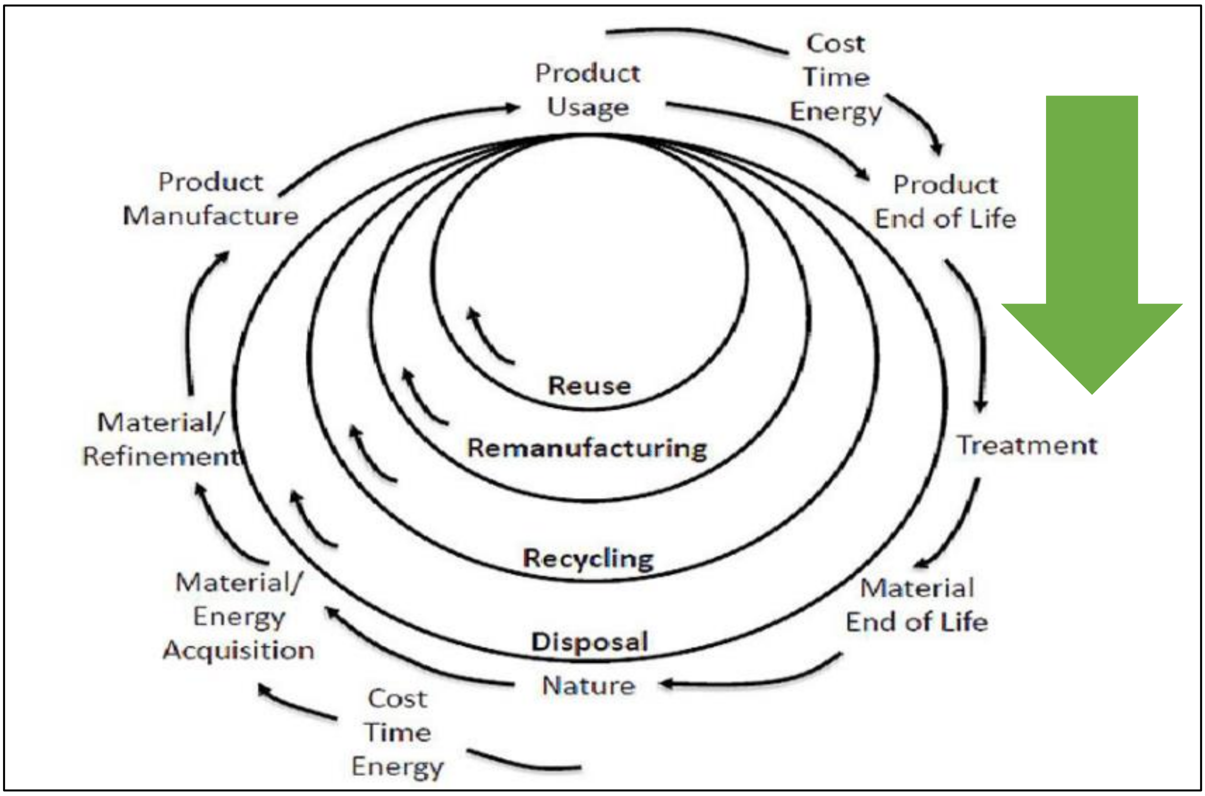


Figure 2.1. The ideal life cycle of products, in the form of a CE. With each successive outer circle, energy and resource demands become greater and less preferable; green arrow = direction of energy flow (Mihelcic et al., 2003)

The concept of CEs is growing in popularity among national governments, non-governmental organisations, and scholars of various fields (Ghisellini et al., 2016; Lieder & Rashid, 2016; Geissdoerfer et al., 2017; Kirchherr et al., 2017; Korhonen et al., 2018). Hundreds of journal articles on CEs have been published, with a significant rise in publishing over the last decade (Geissdoerfer et al., 2017; Kirchherr et al., 2017). Such articles range in topic, from industrial ecosystems to cleaner production (Jelinski et al., 1992; Korhonen, 2001; Stevenson & Evans, 2004). Moreover, as there is plethora of literature composed of fragmented and integrated ideas, CEs as a concept can have several varied definitions (Lieder & Rashid, 2016; Kirchherr et al., 2017; Korhonen et al., 2018). Korhonen et al. (2018) defines CEs as “an economy constructed from societal production-consumption systems that maximises the service produced from the linear nature-society-nature material and energy throughput flow”. Alternatively, CEs can also be defined as a closed-loop industrial economy, in terms of the flow of energy and materials, that is also intentionally regenerative/restorative (Geng & Doberstein, 2008; Yuan et al., 2008; Geissdoerfer et al., 2017). However, despite the abundance of literature on the topics that compose CEs, the literature lacks depth in certain aspects. Additionally, CEs are not without their limitations and issues, both theoretically and practically, as explained in section A.4.2.

A.4.2 Issues with CEs

Georgescu-Roegen (1971) argued that CEs were not possible, as the concept of entropy dictated that "complete" recycling was impossible; therefore, CEs would inevitably become unsustainable, when/if economic growth is left unchecked (Korhonen et al., 2018). Moreover, even if a limit is placed upon the physical scaling of the economy, the associated processes will always require energy and thus generate waste products, before eventually leading to a total system collapse (Daly, 1996; Ghisellini et al., 2016; Korhonen et al., 2018). However, Georgescu-Roegen (1971) assumed that Earth was a finite system. In reality, Earth is an open system that receives renewable—and from an anthropocentric perspective, "infinite"—energy from the Sun (Ghisellini et al., 2016; Korhonen et al., 2018). On the other hand, no matter how cyclical, an "infinite" energy source is far from the only requirement for CEs; there must also be significant and long-lasting changes that encapsulate a holistically green and/or sustainable mindset, from all actors/drivers and intermediaries of sustainability (Ghisellini et al., 2016). CE drivers must address any limitations, such as problem shifting and social/culture-based differences, or potentially become as damaging to society and the environment (Mayer et al., 2005; Mattila et al., 2010; Korhonen, 2018).

All three of the examined CE papers (Lieder & Rashid, 2016; Geissdoerfer et al., 2017; Kirchherr et al., 2017) used the Web of Science database (1950-2015/2016) as the foundation to their respective literature reviews (Appendix D). Geissdoerfer et al. (2017) found that sustainability focuses more on achieving open-ended and broader goals in more flexible timeframes. In contrast, CEs have more specified actors/drivers that aim for closed-loop systems, with a greater focus on environmental and economic priorities (e.g., waste prevention, financial benefits). Furthermore, Geissdoerfer et al. (2017) noted that, while sustainability was regarded as an intrinsic part of CEs, the literature lacks depth in their relation to each other and does not explore a holistic perspective for either concept, with no explicit utilisation of approaches likes MCDM. And if a particular dimension is discussed, it is often simplified or almost ignored in the literature; for example, CEs are often summarised as "inputs→outputs→waste", without consideration to long-term viability, while the social aspects equated to employment opportunities only.

In comparison, Kirchherr et al. (2017) discovered that CE policy has a strong focus on recycling over its other aspects in a 4R framework: reduce, reuse, recycle, and recover (Allwood et al., 2011; Ghisellini et al., 2016). It is also implied from post-2012 literature, that there is a transition away from the aforementioned 4R framework; this is because an increasing number of CE definitions appear to acknowledge the requirement of a holistic perspective on various system scales (i.e. macro-, meso-, and micro-), which may be beyond the scope of a 4R framework. Moreover, it was also determined that approximately 2/3 of CE definitions did not include waste hierarchies, which can prove essential to the interest of the concept for CE drivers/actors and prevent skewed interpretations. Like Geissdoerfer et al. (2017), Kirchherr et al. (2017) noted that the literature establishes a link between CE and sustainable development, and that there is little consideration of the social (and political) aspects of sustainability. Furthermore, Kirchherr et al. (2017) stated that the link between sustainable development and CEs is tenuous, in comparison to Geissdoerfer et al. (2017), with only 12% of the literature definitions having an explicit connection between the two concepts. Therefore, as supported by Lieder & Rashid (2016), the CE literature contains not insignificant research gaps.

Lieder & Rashid (2016) places an emphasis on the economic and environmental dimensions associated with CEs, such as the impacts of pollution and the economic benefits. However, the social dimension is only touched upon in a general sense, though to a relatively greater degree than Geissdoerfer et al. (2017) and Kirchherr et al. (2017). In Lieder & Rashid (2016), there is a strong emphasis on the importance of education and social awareness, but no detailed pathways as to how such social aspects could be carried out. On the other hand, Lieder & Rashid (2016) does acknowledge the fact that CEs require "radical" changes for large-scale implementation and long-term success. Such changes include (but are not limited to) a concurrent methodology, in which CEs are approached from top-down in public institutions and bottom-up in industry, in order to align stakeholder interests. Overall, it is clear from the literature that a truly holistic perspective is sorely lacking, particularly regarding the social dimension. Therefore, future CE applications for sustainability should seek to address all dimensions from an equitable and multi-disciplinary perspective. Well-designed and well-developed MCDM frameworks could be key in rectifying such research gaps, with more in-depth social perspectives and links with other dimensions.

A.5 Biomass

A.5.1 Biofuels

Biomass has a long and extensive history of use in various fields, from transportation to agriculture (Alonso et al., 2010; Gallezot, 2012). As non-renewable resources are depleted, and the negative impacts—such as climate change and rising fuel costs—become increasingly more apparent, society must transition into a more sustainable state, with a greater focus on cleaner, long-term energy sources (Westermann et al., 2007; Chew & Bhatia, 2008; Alonso et al., 2010; Naik et al., 2010; Pacheco-López et al., 2021). Biofuels that are derived from renewable feedstocks, like biomass from municipal solid waste, have gained significant interest as sustainable replacements to conventional fossil-fuels (Alonso et al., 2010; Naik et al., 2010; Senthil et al., 2022; Ye et al., 2024). Unlike vehicular energy sources like solar and hydrogen fuel cells, biofuels are comparatively similar to conventional fuels, in terms of the available support technology and infrastructure. As a result, biofuels can be implemented on a much faster timescale, in addition to their other advantages, albeit mainly from the more sustainable second and third generations of biofuels (Alonso et al., 2010; Naik et al., 2010). Biofuels can be sorted into three main generations: first, second, and third (Naik et al., 2010; Lee & Lavoie, 2013; Senthil et al., 2022). However, there is a fourth generation of biofuels, that are also derived from microalgae, albeit the microalgae are genetically modified (Arpia et al., 2021). But due to the comparative lack of research, fourth-generation biofuels will not be discussed.

First-generation biofuels are highly abundant due to being derived from edible biomass, such as barley and sugarcane, to produce economically viable and sustainable alternatives to conventional fossil-fuels (Naik et al., 2010; Lee & Lavoie, 2013; Senthil et al., 2022; Ye et al., 2024). For example, first-generation biodiesel (with glycerol) is produced as an alternative to diesel, most commonly via the transesterification of fatty acid methyl esters derived from waste cooking oils (Chisti, 2007; Phan & Phan, 2008; Naik et al., 2010; Bhonsle et al., 2022). However, sources of edible biomass for first-generation biofuels face strict and ever-growing rise in food demand, leading to rising costs and thus decreasing cost-effectiveness (Lee & Lavoie, 2013; Srinophakun & Suwajittanont, 202). Consequently, second-generation biofuels are developed from non-edible lignocellulosic biomass—such as low-value municipal solid waste (MSW)—via hydrolysis, gasification, and/or fermentation (Naik et al., 2010; Lee & Lavoie, 2013). In contrast, third-generation biofuels are produced via algae-related biomass, primarily due to high lipid contents, and comparatively rapid growth yields to traditional lignocellulosic sources; this leads to an overall more sustainable and cost-effective production process (Lee & Lavoie, 2013; Alam et al., 2015; Chowdhury & Loganathan, 2019). The advantages of post-first-generation biofuels include less competition for resource availability, enhanced biodegradability, carbon-neutrality (or even being carbon-negative), social mobility, energy security, and environmental-friendliness (Puppán, 2002; Demirbas, 2007; Chew & Bhatia, 2008; Naik et al., 2010). On the other hand, the production of second-generation biofuels involves complex processes and relatively complex raw materials, leading to a whole process design that is not cost-effective (Naik et al., 2010; Chowdhury & Loganathan, 2019; Pulyaeva et al., 2020).

Chew & Bhatia (2008) looked at the pyrolysis of palm oil biomass for a proposed biorefinery in Malaysia, in order to produce environmentally friendly biofuels (Appendix D). The three most important factors toward biofuel production were determined to be the reactor, separation processes, and the catalyst. Chew & Bhatia (2008) placed specific emphasis on catalysis in biofuel production; specifically, the exploration of heterogeneous catalysts. Catalyst separation is an issue for homogeneous catalysts, which has led to more extensive research into the overall capabilities of heterogeneous (nano-)catalysts (Fadhel et al., 2010; Polshettiwar & Varma, 2010; Gawande et al., 2013). Heterogeneous catalysts—such as zeolites (ZSM-5) and mesoporous aluminosilicates (Al-MCM-41)—showed promise due to their porosity and acidity properties, albeit high temperatures appeared to cause potential issues with catalytic thermal stability (Polshettiwar & Varma, 2010; Kalidindi & Jagirdar, 2012; Wang et al., 2012). Chew & Bhatia (2008) also noted the technical and economic barriers involved for biofuel production in the case study; namely, that current biofuel production processes are too different to utilise existing petroleum infrastructure, especially when working with renewable feedstocks. That said, heterogeneous nanocatalysts are cost effective, and increase the rates of transesterification for biofuel production. Overall, there needs to be further research and a better integration of knowledge that constitutes biofuel production, particularly to address the economic and technical barriers. And, if possible, further research should delve into the social dimension of biofuels in relation to sustainable circular bioeconomy (Rebolledo-Leiva et al., 2023; Ye et al., 2024), so that biofuels can become a more holistically sustainable energy resource.

A.5.2 Municipal solid waste (MSW)

Approximately 2 billion tonnes of MSW are produced annually across the globe, and one-third of the MSW is not managed via environmentally friendly means, such as landfill disposal and conventional incineration (World Bank, 2022). Consequently, the mismanagement of MSW has led to severe negative impacts for human society and the environment, including but not limited to ecosystem destruction and groundwater pollution (Gao et al., 2022; Abdollahi Saadatlu et al., 2022). Pyrolysis could be the key to addressing growing MSW concerns, as a relatively environmentally friendly and sustainable means of waste-to-energy conversion (into electricity), waste management, and the production of higher-quality value-added materials/substances (Chen et al., 2015; Wang & Wang, 2019; Song et al., 2020; Gao, 2022). In contrast to conventional feedstocks, MSW offers a sustainably continuous and readily available feedstock supply, with a high efficiency in energy recovery (Chen et al., 2015; Scarlat et al., 2019; Song et al., 2020). Even so, this must be done properly, and there are multi-dimensional limitations associated with MSW.

MSW is heterogeneous and can contain a mixture of waste types, ranging from plastics to wood. Decision-making for maximising viability regarding other key factors—such as reactor type, catalyst(s), residence time, and rates of reaction—can vary greatly, especially as new and/or improved pyrolysis approaches are discovered and explored (Bridgwater & Cottam, 1991; Chew & Bhatia, 2008; Song et al., 2020). Without any prior sorting and separation, reactors may not be able to handle MSW and the derived feedstocks (Chen et al., 2015; Abdel-Shafy & Mansour, 2018). Furthermore, from a social perspective, waste perceptions can hinder its potential in the aforementioned aspects. According to Scarlet et al. (2019), waste is often still viewed as a "nuisance" instead of a resource in most of the EU, despite waste management being an integral part in the shift towards CEs and sustainability (see section A.4). Therefore, it stands to reason that a truly holistic approach needs to be taken in such instances, so that the social dimension—such as the reasonings behind perceptions—is addressed with equal importance to the other dimensions. Appendix D lists a summary of the respective findings on MSW pyrolysis (in blue), from Chen et al. (2015) and Song et al. (2020).

Chen et al. (2015) presented an overarching literature review, that covered the environmental impacts, technologies, outputs, and operation parameters of MSW pyrolysis. There are many factors of pyrolysis that can affect product yields and compositions: feedstock type, rate of heating, final temperature, residence time, and reactor type. However, in terms of outputs, MSW-derived liquid products have been discovered to contain water; therefore, it was recommended that the production of liquid products be avoided. Alternatively, that sustainable and environmentally friendly alternatives are used in pyrolysis for oil production. Even so, the literature acknowledged that there is potential for scale-up in MSW pyrolysis, albeit it varies among MSW pyrolysis technologies. Fixed-bed reactors would not be ideal, due to their inefficiency and non-uniform reactions to MSW feedstocks. Instead, rotary kiln reactors (and to a lesser extent, tubular reactors) may be more preferable in scale-up facilities, primarily due to their flexibility and being relatively low-maintenance. That said, improving the efficiency of rotary kiln reactors should be a priority for scaled-up operations; Chen et al. (2015) recommended a multi-sectional rotary kiln reactor as a viable solution. The main advantages include a higher quality of output production, and a greater likelihood of production reformation. Additionally, while MSW pyrolysis aims to be an environmentally friendly process, there are still improvements that can be implemented; most notably, further characterisation of the outputs, output quality, and the impact(s) on the environment. Simultaneously, there needs to be an integrated holistic approach towards the improvement of MSW pyrolysis. Yet, it is not entirely clear as to how MSW pyrolysis can be affected via a social dimension, or in relation to other dimensions, like the economic and/or environmental.

A novel approach to MSW disposal via pyrolysis was presented by Song et al. (2020): the reduction of iron ore and iron oxide as catalysts to MSW pyrolysis, in a series of fixed-bed reactor experiments. The Kissinger-Akahira-Sunose and Flynn-Wall-Ozawa methods (Kongkaew et al., 2015; Li et al., 2017; Thomas et al., 2020) were used to establish a kinetic analysis model with the parameters, such as activation energy, for MSW pyrolysis. Iron additives had lowered the activation energy for MSW pyrolysis, from 180.32 kJ/mol to 151.76 kJ/mol and 150.18 kJ/mol via iron oxide and iron ore catalysts, respectively (Song et al., 2020). However, pyrolysis conversion could only reach an estimated maximum of 56.01% under optimal conditions (Song et al., 2020). Further research would be required to improve pyrolysis conversion efficiency, albeit the ideal conditions for MSW disposal via pyrolysis could be difficult to determine without extensive testing; partially due to the heterogeneous nature of MSW. Therefore, future MSW pyrolysis testing will also have to involve the improvement of waste sorting and separation, to make the overall process more efficient and cost-effective. Additionally, in order to approach MSW pyrolysis from a more holistic perspective, uncertainties—such as costs, demands, environmental impacts, and/or seasonality issues—could be considered within the context of a supply chain. Instead of approaching MSW pyrolysis from a limited perspective, e.g. solely improving catalytic activity, a supply chain could recontextualise the entire pyrolysis process akin to that of a whole process design philosophy (Sharratt, 2011).

The project requires novel approaches towards the incorporation/enhancement of holistically green sustainability in CPP design and operation. As discussed in regard to MSW, this involves a restructuring on the development and implementation of methodology frameworks. Every factor must be considered, individually and in relation to each other, from a multi-dimensional perspective that utilises whole process design.

A.6 Conclusions

It is widely acknowledged that the environment (and by extension, human society) is at risk of severe multi-dimensional consequences, as the result of unsustainable and/or "unclean" practices. Sustainability has existed as a concept for centuries, but it is only in the past century that humanity started to grow aware of the consequences in various dimensions; socially, economically, and/or environmentally. The most prominent shifts in awareness occurred with the 1949, the release of *Silent Spring* in 1962, and the 1987 Brundtland Report that redefined 'sustainable development'. This was soon followed by the inception of GC in 1991, based on the twelve guidelines set by Anastas & Warner (1998) (Appendix B). Such guidelines state that in GC, waste prevention is a higher priority than remediation and/or research into safer, greener, and more sustainable alternatives. Additionally, while they are indeed intrinsically linked, GC and sustainability are not interchangeable concepts.

In 'GC & Sustainability', the following topics of interest were discussed: CEs and biomass (specifically, biofuels & MSW pyrolysis). The literature review for each GC topic was extensive

(Appendix D), with an explicit awareness of sustainability and/or sustainable development, particularly in regard to their necessity. That said, it is also clear that sustainability is viewed via a mostly economic and environmental perspective; i.e. research into improving the cost-effectiveness of industry methodologies and technologies, while mitigating/preventing the negative environmental impacts. There is little exploration into the social dimension of green sustainability (Mattioda et al., 2020), if any at all, despite the strong social aspects established by frameworks like the SDGs. This is partially due to the relatively undeveloped social databases, in comparison to their environmental and economic counterparts (Mattioda et al., 2020; Rebolledo-Leiva et al., 2023)

Therefore, a greener and more sustainable society will require holistic approaches towards sustainability, in which social databases are better defined and thus no dimension is (comparatively) neglected/underdeveloped. Overall, 'GC & Sustainability' has defined a notable research gap (or series of gaps) within the literature, that the project may be able to address via a novel approach towards sustainability; the integration of MCDM methods with GC and sustainability concepts. Resultantly, the project seeks to provide new and improved pathways to the transition towards green, sustainable societies.

B. Multi-Criteria Decision Making/Analysis (MDCM/A)

B.1 Introduction

Multi-criteria Decision Making/Analysis (MCDM/A) is an instrumental research branch of decision-making theory (Rezaei, 2015). MCDM/A can be divided into two categories: Multi-objective Decision Making (MODM) and Multi-attribute Decision Making (MADM). MODM involves obtaining a set of continuous, competing alternatives—from two or more criteria—that require simultaneous optimisation, with respect to constraints via multi-objective programming; examples include genetic algorithm (GA) and Particle Swarm Optimisation (PSO) (Penadés-Plà et al., 2016; Zavadskas et al., 2019). In comparison, MADM looks at problems that have a limited number of discrete, predetermined alternatives; examples include Complex Proportional Assessment (COPRAS) and its progenitor method, Simple Additive Weighting (SAW) (Penadés-Plà et al., 2016; Zavadskas et al., 2019). Due to their versality and multi-dimensional applications, MCDM methods have been implemented throughout various disciplines, from (municipal solid) waste management, to the production of raw materials (Wang et al., 2009; Behzadian et al., 2012; Ali et al., 2019). MCDM/A can be utilised individually or as part of an integrated model, such as Analytic Hierarchy Process (AHP) or AHP-VIKOR. Resultantly, different MCDM methods can provide varying ranking results based on their methodologies and the decision-makers themselves (Bandyopadhyay, 2020). For example, AHP works by weighing and attaching a rank to each criterion and sub-criterion, that was pre-selected by the decision-makers. Decision-makers can then class and prioritise alternative solutions, based on criteria/sub-criteria rankings, and choose which one is the overall “best” (Stojcic et al., 2019; Fonseca et al., 2021; Kannan et al., 2021; Muhammed et al., 2021).

In more recent years, MCDM methods have enabled decision-makers to approach green sustainability and sustainable development with a more holistic mindset. This is increasingly more important, as human society and the environment may suffer from severe and irreversible consequences (Fonseca et al., 2021; Kannan et al., 2021; Muhammad et al., 2021; Narwane et al., 2021). Posteriori MCDM/A frameworks, in which all sets of possible pathways are analysed prior to the preference establishment (Al-Majali & Zobaa, 2025), could be the key towards achieving a novel, truly holistically green sustainability in CPPs. In this part of the literature review, MCDM methods—(F)AHP, TOPSIS, ELECTRE-III, PROMETHEE-II, and VIKOR—are examined and discussed in terms of their overall history, strengths, weaknesses, limitations, and applications in the literature. The conclusion summarises the findings, and the implications for the project.

B.2 Research Questions

- What are the individual strengths, weaknesses, and limitations of each MCDM method?
- Why is MCDM hybridisation preferred over individual methodologies?
- How was/were method(s) applied in the literature? And why choose and/or integrate the following MCDM methods for this project?

B.3 Analytic Hierarchy Process (AHP)

AHP is one of the most applied MCDM method, with an extensive history of use in various disciplines–from selecting solar sites, to the selection of suppliers of raw materials (Ho et al., 2010; Ali et al., 2019; Nazim et al., 2022)–and for various other purposes, such as conflict resolution (Saaty, 1987; Vaidya & Kumar, 2006). AHP is a hierarchy framework that was first developed by Thomas Saaty in the 1970s with continued refinement even today. It can be broken down into the following basic steps: establish the focus/problem → outline the problem objectives, with consideration to all variables → criteria selection and weightings → sub-criteria selection and weightings (often, but not always) → pairwise comparisons with respect to criterion/sub-criterion and focus → derive the consistency index (CI), normalised values, and consistency ratio (CR) for each alternative (Saaty, 1987; Vaidya & Kumar, 2006; Jamwal et al., 2021).

Flexibility is one of the key attributes of AHP, in addition to its simplicity, ease of use, and its ability—by itself—to make consistent judgements (Saaty, 1987; Ho et al., 2010; Jamwal et al., 2021). However, a certain level of complexity is still required to establish the context of the problem, albeit it also cannot compromise the flexibility of the AHP framework (Saaty, 1987; Vaidya & Kumar, 2006). Due to its high flexibility towards specific decision-maker priorities, an increasing number of studies have adopted seamlessly hybridised AHP frameworks with fuzzy logic (Al-Majali & Zobaa, 2025). FAHP has been integrated and/or used in conjunction with fuzzy variations of techniques like VIKOR, PROMETHEE, and genetic programming; this helps address the limitations of each individual approach and optimises the overall decision-making process (Ali et al., 2019; Wu & Abdul-Nour, 2020; Al-Majali & Zobaa, 2025). However, AHP is not without its weakness or limitations; interdependency among alternatives, data needing to be collected from experience, and overemphasis/underemphasis of criteria by decision-makers (Kumar et al., 2017; Wu & Abdul-Nour, 2020). In the following papers, AHP was utilised as either part of an integrated approach or used in conjunction with other MCDM methods: Awasthi et al. (2017), Ali et al. (2019), and Wu & Abdul-Nour (2020).

B.3.1 Sustainable supplier selection

Awasthi et al. (2017) utilised a two-stage, integrated FAHP-VIKOR approach, for a focal company, with limited quantitative data. The company wanted to select a global main supplier and sub-supplier out of three alternatives for each, based on sustainability criteria (social, economic, environmental, global risks, and relationship quality) and sub-criteria (Appendix E). Criteria weighting was carried out in the first stage via FAHP, while criteria evaluation was given by linguistic assessments from decision-makers, that were subsequently converted into triangular fuzzy numbers (TFNs). Aggregated Individual Judgements (AIJ) was used for score aggregation, before VIKOR was then applied to rank the main supplier alternatives relative to the criteria scores. The same methodology is applied in the stage 2 for the sub-supplier—or more accurately, the (1+n)th-tier supplier—except with only social and environmental criteria/sub-criteria. Awasthi et al. (2017) found that the economic criteria had the greatest weight for the main supplier (0.6), while global risk had the lowest (0.04). In stage 2, environmental (0.662) was given a greater criterion weighting than social (0.337).

Overall, it was determined that the focal company should choose main supplier 3 (or 1) and sub-supplier 3. On the other hand, the study does have its limitations. Due to a pre-determined threshold value, and practical reasons like cost, only a certain number of sub-suppliers could be evaluated in the study. Moreover, the study itself has a lack of quantitative (and real) data, as well as a limited number of decision-making respondents. The study could also be improved upon by the addition of sensitivity analysis and comparisons with other MCDM methods, whether they be integrated or not. And to save on time and computational power, it could be argued that the number of sub-criteria could be reduced, as a large number of sub-criteria can be costly (Wu & Abdul-Nour, 2020)

B.3.2 Urea production

Ali et al. (2019) utilised AHP to assign relative criteria weights, in the context of optimal urea production (Appendix E). Ten questionnaire respondents were selected from the fertiliser industry: three professors, four engineers, and three managers. A linguistic, nine-point scale was also used to decide the best alternative out of three options: prilling, hybrid system, and granulation. In the case of the hybrid system, a 1:1 ratio was assumed between prilling and granulation. The AHP results show that the hybrid system is ranked no.1, followed by granulation and then prilling, for the purposes of profit and process flexibility. On the other hand, in terms of environment, granulation is considered as the best alternative, which is backed up by the results from TOPSIS. Even so, it should be noted that the 'best' alternative for urea production is largely dependent on the aims and objectives of the decision-makers. From an environmentally sustainable perspective, granulation would be the best option, while decision-makers that focus more on profit should choose the hybrid system, particularly since granulation would not be ideal for high-capacity requirements. One of the weaknesses of AHP is that criteria/sub-criteria weights can be overemphasised/underemphasised by respondents, especially for qualitative criteria (Wu & Abdul-Nour, 2020). And, without sensitivity analysis, it may be difficult to determine the robustness of the AHP model (and TOPSIS).

B.3.3 Sewer network planning

Like in Ali et al. (2019), Wu & Abdul-Nour (2020) uses AHP and TOPSIS, but also with the addition of other MCDM methods; PROMETHEE-II and ELECTRE-III. This section focuses solely on the applications of AHP.

Wu & Abdul-Nour (2020) implements MCDM methods to determine the overall best alternative sewer network construction plan out of four options (P1-4), with the aim of reducing rainfall flow to a pumping station. Eight professionals were chosen for this project: a project manager, two sanitary engineers, an environment/meteorological expert, two civil engineers, and two road operators. AHP was applied manually, as it is not (nor based on) a complex algorithm. Due to the presence of five criteria (construction cost, potential for future profit, dynamic performance, maintenance cost, and environmental impact), ten pairwise comparisons had to be carried out to derive the criteria weights. Additionally, as there are four alternatives, a total of thirty pairwise comparisons (six for each of the five criteria) are required, before the Delphi method converts the data into six pairwise comparison matrices. Throughout this process, it is ensured that pairwise comparisons are consistent.

The AHP results discovered that 'dynamic performance' has the greatest weighting (0.2349), while 'environmental impact' has the lowest (0.1441). According to the final AHP scores, P2 is the highest-ranked alternative, followed by P1, P3, and P4. In regard to the approach itself, AHP was noted by decision-makers as "accurate" and "efficient", although the strenuously long process of making numerous pairwise comparisons had an adverse effect on decision-maker confidence. Additionally, while the final AHP scores were shown to be consistent, greater emphasis was placed upon the more positive criteria weights (i.e., profit and dynamic performance) than the negative with AHP; this created a contrast in weighting consistency to the other MCDM methods implemented in the paper. As mentioned in section B.3.2, AHP struggles with consistency when dealing with non-numerical data, possibly because subjective opinions—particularly given repeatedly, known as decision fatigue—is arguably more strenuous on the decision-maker than using pure numerical data. The paper suggests overemphasis/underemphasis of criteria could be attributed to the typically used AHP 1-9 scale (Saaty, 1987); therefore, future studies may want to take advantage of AHP's flexible nature and design a different point scale; e.g., five-point or 100-point.

B.4 Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS)

TOPSIS was first developed and presented by Hwang & Yoon in 1981 (Chen, 2000; Opricovic & Tzeng, 2004; Behzadian et al., 2012; Wu & Abdul-Nour, 2020). Alternatives are evaluated and chosen based on their respective distances from the positive-ideal solution (i.e. maximisation of positive criteria; minimisation of negative criteria) and the negative-ideal solution (i.e. maximisation of negative criteria; minimisation of positive criteria) (Behzadian et al., 2012; Wu & Abdul-Nour, 2020; Al-Majali & Zobaa, 2025). The key advantages of TOPSIS are that decision-makers do not need to implement numerous inputs, high computational efficiency, and that the outputs are relatively straightforward to read and understand (Kumar et al., 2017; Wu & Abdul-Nour, 2020).

TOPSIS also utilises criteria information to its fullest, without the requirement of independent criteria, albeit this is only possible when all information is both available and accurate (Kabir et al., 2014; Kumar et al., 2017). Moreover, while there are advantages, TOPSIS does have two notable weaknesses: the requirement of vector normalisation for multi-dimensional problems (Kabir et al., 2014; Wu & Abdul-Nour, 2020), and the relative importance of the distances for the ideal solutions not being properly considered (Opricovic & Tzeng, 2004; Kumar et al., 2017). Additionally, a potential weakness/limitation to TOPSIS, is the use of crisp data values. Real-life scenarios are often fraught with uncertainty and relativity (Chen, 2000), which is why the incorporation of fuzzy logic to TOPSIS and other ranking methodologies has become more popular (Kabir et al., 2014; Balioti et al., 2018). Perhaps, the combined implementation and/or integration of crisp and fuzzy data in TOPSIS could be the ideal solution in holistically green sustainability.

In the following sections (B.4.1-.4.4), several papers, regarding the application of TOPSIS and other MCDM methods, are discussed in relation to TOPSIS.

B.4.1 Urea production

Section B.3.2 discusses the application of AHP in Ali et al. (2019) for optimised urea production. TOPSIS was also implemented to evaluate and rank the alternatives to select the optimal choice, which can vary depending on the aims of the decision-makers. The results from AHP and TOPSIS illustrate that granulation is the optimal method of urea production, from an environmental perspective (Appendix E). Contrastingly, in terms of optimising profit and reliability, prilling is regarded as the best alternative. However, it should be noted that AHP had influenced TOPSIS results, likely due to the overemphasis/underemphasis of criteria. Specifically, prilling is the no.1-ranked alternative, from an environmental perspective, despite its relative closeness to the negative-ideal solution. Overall, TOPSIS (and AHP) calculated that prilling was the optimal alternative for urea production. But like with AHP, the lack of sensitivity analysis for TOPSIS places some doubt upon the robustness of the approach and its results.

B.4.2 Amazon book sales

Bandyopadhyay (2020) studied data on Amazon book sales with the following MCDM methods: TOPSIS, Multi-attribute Utility Theory (MAUT), and Measuring Attractiveness by a Categorical Based Evaluation Technique (MACBETH). Bandyopadhyay (2020) evaluated the three methods, in terms of algorithm complexity, and found that they are share similar levels of complexity. Twenty book titles acted as the alternatives, in which the ranked top 10 would be chosen for purchase. Book criteria included no. of pages, rating, and price with the following respective weightings from decision-makers: 0.28, 0.39, and 0.33. Using TOPSIS to rank the alternatives, no.9 was deemed the optimal alternative. In comparison to MAUT and MACBETH, only the former shares the no.1 choice for overall best alternative. Even so, like MACBETH, MAUT rankings differed greatly to rankings via TOPSIS; this can be attributed to the value scaling present in TOPSIS, and how criteria are not treated separately. Due to the fact that its methodology involves the ranking of alternatives, based on distances from positive-ideal and negative-ideal solutions, TOPSIS is arguably the more dependable, if not overall superior, MCDM out of the three implemented in Bandyopadhyay (2020), which is illustrated by the criteria score aggregation. That said, the paper could have applied sensitivity analysis to verify robustness for the applied Posteriori MCDM methods.

B.4.3 Sewer network planning

Like AHP, TOPSIS is not based on a complex algorithm; therefore, it had been manually employed for this study (Wu & Abdul-Nour, 2020). That said, Excel and Python coding language can be used for greater ease (Nazim et al., 2022). Delphi method was applied three times, before participants had to finalise their assigned criteria weights. Because criteria scores for each alternative had to be expressed with the same measurement unit via vector normalisation; a 10-point rating system, where 1 = "extremely poor performance" and 10 = "excellent performance". Criteria scores were then averaged into the final scores. The aforementioned process was repeated for each alternative (P1-4) presented in the study, followed by the construction of a decision matrix of criterion averages. Out of the four alternatives, it was determined that P2 had the highest averaged scores for maintenance cost, construction cost, and environmental impact. In comparison, P3 scored highest in potential future profit and dynamic performance (Appendix E). On the other hand, by using TOPSIS, the final rankings were obtained based on relative closeness, in descending order; P1, P2, P3, and P4. Therefore, TOPSIS suggests that P1 and P2 would be the optimal alternatives, as ranked first and second place, respectively.

In contrast, the results are inverted with AHP (section B.3). Moreover, TOPSIS was regarded by respondents as "less complex" in comparison to the number of pairwise comparisons required in AHP; this was the reason why TOPSIS criteria weights were used for the other two MCDM methods in Wu & Abdul-Nour (2020)—ELECTRE-III and PROMETHEE-II—than the weightings from AHP. On the other hand, the required implementation of vector normalisation to differing criteria can lead to potential decision-maker biases for the final criteria scores, particularly for quantitative data, as well as reducing the overall accuracy of rankings (Opricovic & Tzeng, 2004; Kabir et al., 2014; Wu & Abdul-Nour, 2020).

B.4.4 Quality of Life at different spatial levels

Vakilipour et al. (2021) evaluated quality of life at three spatial levels for districts and sub-districts in Tehran, Iran, from a holistic perspective. The paper employed four MCDM methods—TOPSIS, ELECTRE, VIKOR, and SAW—with numerous criteria and sub-criteria (Appendix E). The three spatial levels were as follows: 1) comparisons of subdistricts between two districts (Districts 6 & 13); 2) comparisons of sub-districts within each district; 3) overall district comparison. To ensure that the most suitable variables had been selected, at least for socio-economic criteria, a correlation matrix between variables was established for factor analysis; if variables shared no sufficient correlation, they would be discarded from the study. Factor analysis was also evaluated via the Bartlett sphericity test and the Kaiser-Meyer-Olkin (KMO) co-efficient. If KMO<0.5, the data is unsuitable for factor analysis; for the Bartlett test, if p-value<0.05, reject the null hypothesis, i.e. no differences in variance among groups (Lim & Loh, 1996; Rossoni et al., 2016). The next step was component extraction via Principal Component Analysis (PCA); specifically, the extraction of those that could be behind the data's maximum variance. Components were assigned eigenvalue criterion, with >1 values representing significant components (Mackiewicz & Ratajczak, 1993). Finally, a matrix of variables and components had to be constructed. Variable-component relationships were represented numerically via factor loadings; values equal or greater than 0.71 were regarded as "excellent", while 0.63-0.71 as "very good", and 0.55-0.63 as "good". Any factor loadings between 0.33-0.45 (or lower) were regarded as "weak".

TOPSIS (as well as VIKOR and ELECTRE) determined that sub-district 9 of District 13 was the highest ranked, and each sub-district 9 was highest rank for both districts. In terms of method stability, TOPSIS was ranked the second most stable, only being comparatively less so than SAW. Overall, the method was also noted to be similar to ELECTRE and SAW, in terms of the decision-making and similarity of alternative rankings. As evidenced in the study, method comparisons help ensure that results are more precise, more accurate, and more effective in the decision-making process. By itself, TOPSIS is not enough, which is why the incorporation of other MCDMs is arguably essential. On the other hand, Vakilipour et al. (2021) argues that, if the scope of study is relatively small/limited, MCDM methods will become similar enough for the weaknesses (of TOPSIS, or any individual MCDM method) to no longer be too detrimental to the decision-making process.

B.5 Elimination & Choice Expressing the Reality (ELECTRE)

The ELECTRE family are outranking methods that rely on preference-based data aggregation, using pairwise comparisons and outranking relations to derive the optimum alternative (Pohekar & Ramachandran, 2004; Cinelli et al., 2014; Kumar et al., 2017; Wu & Abdul-Nour et al., 2020; Vakilipour et al., 2021). With the process of establishing the outranking relations, indifference thresholds, concordance indices, and discordance indices are applied, which serve to validate the results and removes poor criteria (Cinelli et al., 2014; Kumar et al., 2017; Vakilipour et al., 2021). Concordance and discordance indices calculate to what degree that option *a* is (at a minimum) as good as option *b* or vice versa, respectively (Pohekar & Ramachandran, 2004; Wu and Abdul-Nour, 2020). Unlike AHP or TOPSIS, the ELECTRE method cannot be easily summarised into straightforward steps (Pohekar & Ramachandran, 2004). Even so, the ELECTRE family does have its unique advantages, which is why the method is utilised throughout various disciplines, particularly in the field of energy planning via ELECTRE-III (Beccali et al., 1998; Pohekar & Ramachandran, 2004). Furthermore, from a sustainability standpoint, it is argued that ELECTRE is an ideal method for the enforcement of strong sustainability (Cinelli et al., 2014).

The ELECTRE family is capable of handling discrete, heterogenous criteria, whether they be quantitative or qualitative (Pohekar & Ramachandran, 2004; Cinelli et al., 2014; Kumar et al., 2017). ELECTRE also has the capability to accept trade-off(s), i.e. compensation, albeit the degree of which depends on the decision-maker(s) (Cinelli et al., 2014; Vakilipour et al., 2021). Moreover, ELECTRE—while more complex than AHP—is in some ways more reliable, as alternative comparisons can be made, even when there are no specific preferences (Vakilipour et al., 2021). And unlike TOPSIS, where criteria data can be warped by vector normalisation, ELECTRE has the option to avoid compensation (Wu & Abdul-Nour, 2020). On the other hand, this involves numerous technical parameters/objectives that require decision-makers to understand specialised knowledge (Kumar et al., 2017; Wu & Abdul-Nour, 2020). This is not helped by the lack of user-friendliness associated with ELECTRE, though certain software platforms—like ChemDecide (section B.5.1)—can mitigate the issue, so long as decision-makers know how to use it/them (Gilliams et al., 2005). Said software platform enables ELECTRE to consider a greater number of criteria than AHP; however, like AHP and VIKOR, rank reversal can become a significant problem with too many criteria, or the removal/addition of criteria (Saaty, 1987; Cinelli et al., 2014; Papathanasiou, 2021). Sections B.5.1-.5.2 examine the implementation of ELECTRE alongside other MCDM methods.

B.5.1 Sewer network planning

ELECTRE—specifically, ELECTRE-III—was one of the MCDM methods applied in Wu & Abdul-Nour (2020). A decision framework was modelled using ChemDecide, that was developed by Hodgett (2016). ChemDecide consists of four tools: a way to structure the problem, and three analysis tools from the three MCDM methodologies (ELECTRE-III, for example). The former involves the user setting an overarching goal, the alternatives, and the criteria, while the latter tools inputted the criteria weights and alternative performances. However, largely due to its time-consuming nature, the project manager acted on behalf of all eight professional participants to input their perspectives into the ELECTRE-III analysis tool. That said, the project manager had stated that the incorporation of ChemDecide as part of decision-making was positive. Additionally, ChemDecide aided in organisation and structure, as well as understanding the relations between inputs, outputs, and factors.

However, ELECTRE-III had not displayed specific alternative scores as part of the results. Instead, the results showed that P2 and P1 were both deemed the optimal alternative, depending on ascending or descending order, respectively. Therefore, the results from ELECTRE-III could not give a conclusive decision, in comparison to the other MCDM methods, which gave only one alternative—either P1 or P2—as the overall best alternative. On the other hand, unlike in TOPSIS, quantitative values could be used; this meant that alternative scores for ELECTRE-III were more consistent, even if less conclusive.

B.5.2 Quality of Life at different spatial levels

Out of the 24 sub-districts, ELECTRE, TOPSIS, and SAW had all assigned the top rank to District 13, sub-district 9. However, there were several ranking differences when comparing ELECTRE to the aforementioned methods (and VIKOR). For example, when considering all 24 sub-districts, District 13, sub-district 12 was assigned rank 6 in ELECTRE vs. ranks 5 and 11 in TOPSIS and SAW, respectively. The resulting inconsistences among MCDM methods can be attributed to the methodologies, as well as the variations in designated criteria values. Even so, there are still some similarities that need to be considered. Vakilipour et al. (2021) derived percentage values that pertained to identical rankings shared among MCDM methods, when evaluating all 24 sub-districts; 16.7% for ELECTRE and VIKOR, and 12.5% for ELECTRE and TOPSIS. Moreover, it was discovered that all MCDM methods had a >0.8 positive correlation at a 95% confidence level. In terms of stability, however, only VIKOR was less stable than ELECTRE. Nevertheless, despite the variations in results, ELECTRE did provide an overall answer on the best sub-district in each district and among sub-districts, in conjunction with the other MCDM methods utilised in the paper.

B.6 VIKOR

VIseKriterijumska Optimizacija I Kompromisno Resenje was developed by Serafim Opricovic in 1979, with its first application in 1980, for the multi-criteria optimisation of complex systems (Opricovic & Tzeng, 2007; Kannan et al., 2021; Vakilipour et al., 2021). VIseKriterijumska Optimizacija I Kompromisno Resenje is Serbian and translates into ‘Multi-Criteria Optimisation and Compromise Solution’ (Chen, 2022; Türegün, 2022). One of the advantages of ‘VIKOR’ (coined in 1990 from the original Serbian phrase; Türegün, 2022) is that it relies on both quantitative data and personal (qualitative) viewpoints (Kannan et al., 2021; Vakilipour et al., 2021; Al-Majali & Zobaa, 2025). This results in the generation of one or more compromise solution(s)—from the ideal solution—that can enable a more accurate reflection of decision-maker opinions (Kannan et al., 2021; Papathanasiou, 2021; Vakilipour et al., 2021; Al-Majali & Zobaa, 2025). Hence, VIKOR is one of the more popular choices of MCDM methods, commonly applied via MATLAB, particularly for supplier selection and situations in which decision-makers cannot yet convey their target objectives (Shemshadi et al., 2011; Vakilipour et al., 2021). Alternatives/Pathways are ranked and sorted based on "closeness" to the positive- and negative-ideal solutions (Opricovic & Tzeng, 2007; Liu et al., 2014; Awasthi et al., 2017; Kumar et al., 2017), quite similar to TOPSIS, in respect to non-commensurable and (potentially) conflicting criteria that can be compromised for the sake of conflict resolution (Opricovic & Tzeng, 2004; Shemshadi et al., 2011; Liu et al., 2014). The obtained 'compromise' result represents maximum "group utility" for the "majority", and the minimum for "individual regret" from what is regarded as the opposing side (Shemshadi et al., 2011; Al-Majali & Zobaa, 2025).

However, as an updated version of TOPSIS, VIKOR utilises linear normalisation to remove criterion units; therefore, normalised values are independent of the criterion's evaluation unit (Opricovic & Tzeng, 2004; Opricovic & Tzeng, 2007). Furthermore, a key difference between TOPSIS and VIKOR, is that the optimum alternative for the former method may not necessarily equate to closeness to the ideal solution like with the latter (Opricovic & Tzeng, 2004). Sections B.6.1-.6.3 examine papers that utilise VIKOR, in addition to other MCDM methods.

B.6.1 Sustainable supplier selection

Awasthi et al. (2017) had utilised an integrated FAHP-VIKOR approach to decision-making for selecting a global sustainable supplier and sub-supplier. Fuzzy VIKOR was implemented to rank supplier alternatives relative to the criteria weighting via FAHP (section B.3.1). Supplier (and sub-supplier) alternatives were assigned linguistic criterion assessments ratings with corresponding TFNs to form a fuzzy average decision matrix. The TFNs were then defuzzied into crisp values via Eq.1, where a_n is a crisp numerical value. Example: criterion *a* with the fuzzy value of '1'—i.e. "equally preferred important to criterion *b*"—would have a TFN of (1,1,3) and a crisp value of 4/3 or 3.33 (2 d.p.).

$$a = \frac{a_1 + 4a_2 + a_3}{6} \tag{1}$$

The best and worst values (f_j^+ and f_j^-, respectively) were then calculated, in addition to the Q_i, R_i, and S_i values. As explained in section B.3.1, the results suggest that the optimal main supplier alternative would either number 1 or 3, while the optimal sub-supplier would be number 3. But like with the FAHP, the robustness of fuzzy VIKOR could have been evaluated with sensitivity analysis and/or uncertainty analysis. It could also be argued that more quantitative data should have been acquired for the study. On the other hand, this could have complicated and compromised the VIKOR methodology, as more data could mean more conflict than VIKOR can handle; it could lead to an increasing difficulty in applying the VIKOR method itself. Moreover, the inclusion of more quantitative data would lead to the required implementation of (potentially) time-consuming and costly modifications, in order to create a more reliable real-time model (Kumar et al., 2017).

B.6.2 Solar site selection

Kannan et al. (2021) had utilised a hybridised MCDM methodology: VIKOR with Gray Relational Analysis (GRA) and Best-Worst Method (BWM). The aim of the paper was to select the optimal locations, in terms of their overall sustainability, for solar photovoltaic (PV) site placements, in the South Khorasan province of Iran. BWM was chosen to assign criteria weights—criteria and sub-criteria are listed in the table—over other methods, such as AHP, due to the fewer required comparisons, and the lower likelihood of potential bias from decision-makers on the weightings. For the solar site location rankings, it was determined that Birjand, the capital of South Khorasan, would be the optimal location for solar site installation. Additionally, the criteria weights suggest that decision-makers place the most value on the following sub-criteria: construction cost, initial investment, and ecosystem destruction. The importance of the first two sub-criteria can be partly attributed to Iran's economic vulnerability, not just the decision-makers' aim of promoting sustainable energy production. Therefore, for other case studies also studying solar PV sites, it is important to note that the surrounding environment(s) can have a significant impact upon decision-maker thought processes.

The potential site locations were ranked via VIKOR and GRA, in addition to sensitivity analysis via 1000 Monte Carlo Simulation-Based (MCSB) runs, to test the robustness, consistency, and reliability of VIKOR and GRA. To compare and evaluate robustness, two function values had to be derived first; f_1, the no. of changes in alternative rankings, and f_2, the no. of changes in their positions. The method with less variance in f_1 and f_2 (i.e. VIKOR) was deemed less sensitive; therefore, its solutions were considered to be more reliable to use in the study than GRA. If feasible, particularly in terms of resources, future studies could improve the hybridised MCDM model by including more criteria and sub-criteria, as well as incorporating sensitivity analysis for each criterion. Different MCDM methods could also be integrated into the hybrid model, so long as potential improvements do not significantly conflict with the new methods; for example, a greater number of criteria/sub-criteria (and thus, pairwise comparisons) would mean that AHP would not be suitable.

B.6.3 Quality of Life at different spatial levels

In contrast to SAW and TOPSIS, sub-district 1 of District 6 was the highest ranked via VIKOR in Vakilipour et al. (2021). Moreover, VIKOR assigned several different sub-district rankings for Districts 6 and 13 when ranked independently, compared to SAW and TOPSIS; however, the no.1 sub-district for District 13 was shared by all methods. As explained in section B.5.2, Vakilipour et al. (2021) derived percentages for the proportion of the same rankings shared among MCDM methods, where it was found that 16.7% of VIKOR rankings were identical to SAW and ELECTRE (16.7% for each method, for the overall rankings). Therefore, it can be stated that VIKOR, SAW, and ELECTRE have similar performances. That said, VIKOR was calculated to have the lowest stability of the methods, which means that VIKOR has a comparatively greater likelihood of results being changed by scale modifications.

B.7 Preference Ranking Organisation Method for Enrichment Evaluations (PROMETHEE)

The PROMETHEE family is a group of outranking methods that was first introduced by J.P. Brans in 1982, before being further developed by Vincke & Brans in 1985 (Behzadian et al., 2010; Abedi et al., 2012; Wu & Abdul-Nour, 2020; Jamwal et al., 2021). Certain conditions must be met, before PROMETHEE can be properly applied; assigned criteria weights are flexible, the process is understandable to decision-makers, and degree(s) of differences among criteria must be considered (Cinelli et al., 2014). So long as the aforementioned conditions are met, PROMETHEE can be used to rank a set of alternatives, in respect to often conflicting criteria via pairwise comparisons, not unlike AHP (Behzadian et al., 2010; Abedi et al., 2012). However, in comparison to AHP, PROMETHEE was shown to be relatively easier to use and implement (Gilliams et al., 2005). All of the PROMETHEE methods—I-VI and GDSS—have been utilised for decision-making in various disciplines, with each PROMETHEE method having its own strengths (Behzadian et al., 2010; Wu & Abdul-Nour, 2020; Jamwal et al., 2021). For example, PROMETHEE-II is commonly implemented, particularly in green sustainable research fields, as it allows decision-makers to carry out the complete ranking of alternatives (Abedi et al., 2012; Cinelli et al., 2014; Jamwal et al., 2021).

PROMETHEE-II was stated to be more stable than ELECTRE and more reliably provide decisive and relatively nuanced ranking results (Brans et al., 1986; Wu & Abdul-Nour, 2020; Al-Majali & Zobaa, 2025). It can also be applied with grey, i.e. missing/insufficient, information that does not need to be normalised, unlike TOPSIS or ELECTRE (Wu & Abdul-Nour, 2020). Even so, PROMETHEE has its weaknesses and limitations. A potential weakness of the PROMETHEE methods, is the assumption that criteria can be appropriately weighted by the decision-maker(s); in addition to potential bias, decision-making becomes increasingly more difficult and fatigue-inducing with a greater number of criteria and sub-criteria (Behzadian et al., 2010; Kumar et al., 2017). Additionally, implementing PROMETHEE can be incredibly time-consuming, partially due to the complexity of the algorithm, albeit this can be mitigated by certain software platforms, e.g. Smart Picker Pro (Kumar et al., 2017; Wu & Abdul-Nour, 2020). Sections B.7.1-.7.4 discuss papers that implement PROMETHEE, either integrated with other MCDM frameworks or simply by itself.

B.7.1 Sewer network planning

To make things easier for the decision-makers, PROMETHEE-II was employed in Wu & Abdul-Nour (2020) via Smart Picker Pro, a specialised software platform. The decision-makers were therefore able to model their sewer network problem in a step-by-step process. And, as with ELECTRE-III from section B.5.1, the project manager had represented the eight professional participants by inputting the following: alternative performances, preference parameters (i.e. whether a criterion is beneficial or a cost), and criteria weights. The results generated from Smart Picker Pro determined that P1 had the overall best performance in each criterion, with not a single “bad” performance. In contrast, P2 was a firm second place, while P3 and P4 offered far worse performances based on their negative net outranking flows.

Overall, PROMETHEE-II was regarded as easy and time cost-effective to apply with software aid, like ELECTRE-III. Furthermore, because it could utilise true (i.e. non-normalised) experimental data, PROMETHEE-II was consistent in its rankings. However, unlike ELECTRE-III, PROMETHEE-II managed to provide a conclusive optimal alternative (P1 vs P1 and/or P2). This was the main reason as to why Wu and Abdul-Nour (2020) states that decision-makers preferred the PROMETHEE-II method, in addition to its other aforementioned advantages.

B.7.2 Chemical vehicle exhaust emissions

Beynon & Wells (2008) is a non-country specific paper that had aimed to evaluate motor vehicles, based on their chemical exhaust emissions, in order to determine the minimal changes required to boost individual vehicle rankings. A PROMETHEE-based methodology with the Gaussian preference function was employed with a sample size of eight motor vehicles. The small vehicle fleet was chosen to represent what would be available for the average "family buyer", with the following included in each vehicle: automatic gearbox, nominal 2.01 capacity, and a petrol engine. Diesel vehicles were excluded on the basis that such vehicles are only common in Europe. Four criteria were selected (in g/km): carbon monoxide (CO), hydrocarbons (HCO), carbon dioxide (CO_2), and nitrogen oxides (NO_x). In the first set of vehicle rankings, all criteria weights were equal, i.e. 0.25x4.

Under such conditions, PROMETHEE calculated the net outranking flows and subsequently assigned the highest rank to the Toyota RAV4. Contrastingly, the Volkswagen Sharan was assigned the lowest ranking. Therefore, engineering modifications to the manufacturer for the Volkswagen Sharan were suggested, depending on what vehicle the manufacturer wants to equal or outrank. For example, in order to jump up to no.6 in ranking, the Volkswagen Sharan would need a (minimum) reduction of 21.4 g/km in CO_2 emissions, when CO_2 is regarded as the most important variable. When CO_2 was assigned the greatest criteria weight, Citroen C4 was always ranked no.1 instead of the Toyota RAV4. The Toyota RAV4 was ranked no.2 or no.3, depending on the criteria weights, because of the C4's low CO_2 emissions. Moreover, a degree of rank reversal for other vehicles—such as the Volkswagen Beetle—was noted in the study with varying criteria weights, which further highlights the sensitivity of the PROMETHEE method. Such sensitivity must be considered, particularly with emission-related research, as it is unlikely that equal weightings would always be suitable with criteria.

B.7.3 Recycling plant installation

Queiruga et al. (2008) had applied PROMETHEE with the Gaussian, linear, and linear with indifference preference functions. The study aimed to determine the optimal Spanish municipality alternative to install Waste Electrical and Electronic Equipment (WEEE) recycling plants. PROMETHEE has a history of being utilised to resolve decisions that involve selecting the most appropriate location(s) for facilities, such as hydroelectric power stations and waste dumpsites (Mladineo et al., 1987; Briggs et al., 1990; Vuk et al., 1991). Criteria and sub-criteria were chosen based on an in-depth survey of WEEE recycling plant characteristics and Spanish municipalities. The alternative municipalities had to have a population that exceeded 23,000 people; therefore, 242 municipalities were deemed suitable for ranking. Thirty experts were selected to evaluate the criteria on a 1-10 scale and/or add criteria, with statistical data from official databases and a questionnaire.

However, although the questionnaire had managed to cut down the number of sub-criteria from seventeen to ten, eighteen of the thirty potential participants did not respond to the questionnaire. The twelve respondents consisted of the following: three electrical appliance manufacturers, one university student, one environmental policymaker, three scrap merchants, and three WEEE recycling plant experts. If the other eighteen individuals had responded as planned, it can be argued that the study could have provided a more accurate and reliable representation of criteria weights, as well as changed the overall municipality rankings. Even so, the use of official statistical databases for the averaged criteria weights ensured a relatively high level of accuracy, if not reliability for the study. On the other hand, criteria information for a number of the municipals did not exist. Therefore, the study had to somewhat rely on aggregated data, which arguably inhibits the reliability of the study. The averaged weighting for each criterion and sub-criterion were assigned by the decision-makers, with infrastructure (0.5) being regarded as the most important criteria, followed by economic (0.29) and legal (0.21).

The results derived the top 20 municipalities, with many of the twenty found to be located around Andalucía and Madrid, regardless of the preference function, albeit the results are not tabulated in the paper. This highlights the overall robustness of the PROMETHEE method, since rankings were not significantly shifted based on criteria weights or preference function. In regard to the alternatives, those that were located in larger cities were preferred over those in autonomous communities, due to factors such as infrastructure availability, population size, and/or population density. That said, being the top in one variable is not everything; alternatives that have lower personnel and land costs, such as Sevilla (no.2), were assigned a higher overall ranking (with Gaussian) than Madrid (no.17), which had the highest population of the alternatives. Furthermore, as the criteria scores were incredibly close, Sevilla would be an arguably superior alternative to the assigned no.1, Huelva, when considering the former's higher score in infrastructure. It is ultimately up to what the decision-maker(s) aim to achieve in the alternative selection process.

B.7.4 Copper mining

Abedi et al. (2012) had applied PROMETHEE-II with the Gaussian and V-shape with indifference functions, as a means to evaluate porphyry copper deposits in Iran; specifically, from 21 previously drilled, economically viable boreholes in the Now Chun deposit, located in the Kerman province. A mineral prospectivity map was constructed out of thirteen data layers, with the layers serving as the sub-criteria (Appendix E). The Delphi method was employed by decision-makers for criteria weights, before the net outranking flows were calculated. Once the net outranking flows were derived, a complete ranking of the 21 boreholes could be provided, ordered from best to worst. Said 21 boreholes were assigned qualitative rankings from 1-5, where higher values corresponded to higher rankings; e.g., 5="extremely good" and recommended for additional drilling. PROMETHEE-II determined that six boreholes and their surrounding areas—no.1, no.5, no.6, no.9, no.10, and no.15—should be recommended for further study. On the other hand, outside of the aforementioned areas, additional drilling was not recommended within the study area.

But to 1) ensure that borehole misclassification was not a significant issue, and 2) check the robustness of PROMETHEE-II, Abedi et al. (2012) derived a value for the Correct Classification Rate (CCR), where the CCR compares estimated with actual class values. A confusion matrix was established, from which the sum of diagonal components was divided by the total no. of boreholes (N=21). The CCR for this study had been calculated to be 0.4286; therefore, the authors had deemed PROMETHEE-II as a reliable and powerful methodology for mineral prospectivity mapping. However, since CCR=1 when the estimated and actual class values are all the same, it can be argued that 0.4286 is too low for PROMETHEE-II to be classified as "reliable". Abedi et al. (2012) explained that fewer classes could increase the CCR value, with two classes being sufficient; non-deposit and prospect-deposit. On the other hand, using two classes for the copper deposits would only provide a binary answer; beyond that, it would be unclear to what degree each borehole (and the surrounding area) has potential for additional drilling.

B.8 Conclusions

This project aimed to integrate MCDM methods into CPPs, in a holistic approach towards green sustainability and sustainable development. The literature shows that MCDM has had extensive applications in various fields across the world, from solar site selection in east Iran, to selecting the optimal installation location(s) for WEEE plants in Spanish. Moreover, each MCDM method has its strengths, weaknesses, and limitations. AHP is by far the most common MCDM method in the literature, with its flexibility and ease of application as its key strengths, albeit criteria are interdependent and may receive unequal weightings. In comparison, TOPSIS is similarly easy to apply, and independent criteria are not required; however, criteria data can be altered by the required vector normalisation. Unlike TOPSIS, VIKOR uses linear normalisation for the criterion units, and the subsequent normalised values can remain independent from the criterion units. Additionally, VIKOR can provide a more accurate representation of decision-maker viewpoint(s) via compromise solutions. That said, conflicts can more easily destabilise VIKOR and lead to inaccurate results, compared to the other MCDM methods. ELECTRE-III is stated to best embody the concept of strong sustainability, albeit the MCDM method itself is overall difficult to implement without pre-existing expertise, even with the aid of software.

For this reason, PROMETHEE-II appeared to be the overall superior outranking method to ELECTRE-III; the former provides more conclusive and consistent optimal alternative rankings, grey data can be utilised, and the data itself does not require normalisation. On the other hand, PROMETHEE-II can lack versatility, and individual applications can be less reliable in comparison. The outranking method can also be difficult to implement without software aid, albeit not to the extent of ELECTRE. To mitigate the individual limitations, MCDM methods were integrated for this project, like the use of AHP-VIKOR by Awasthi et al. (2017). This project integrated three MCDM methods: (F)AHP, VIKOR, and PROMETHEE-II. FAHP is incredibly adaptable, easy to use, and presents a clear hierarchical structure. The integration of VIKOR provided a more accurate representation of decision-maker viewpoints via compromise solutions, while also removing criterion units in a way that did not distort criteria data. PROMETHEE-II could further improve the integrated MCDM framework and vice versa. PROMETHEE-II's lack of versatility could be mitigated by the high adaptability and flexibility of FAHP, while the compromise solutions from VIKOR maximised the conclusiveness and reliability of the results.

Moreover, as it was notably absent (or simply not mentioned) in most of the researched literature, the project chose to incorporate sensitivity analysis. Sensitivity analysis enabled the project manager and/or decision-makers to assess the robustness of the methodology. Additionally, the MCDM framework must properly account for all dimensions of green sustainability in chemical process plants. The literature highlighted a key weakness in previous sustainability studies: a notable lack of depth, if not neglect, for the social dimension of sustainability as a whole. Therefore, the project had sought to treat all criteria from (more) balanced, holistic perspectives.

C. Chemical Process Plants

C.1 Introduction

Chemical processes are composed of various stages and steps (Sharratt, 2011; Hodgett, 2016), which is why secure and efficient process design is essential in the chemical industry (Misra et al., 2002; Ramzan et al., 2006; Sharratt, 2011; Pasman et al., 2020). The chemical processing industry itself is a holistic cornerstone to modern society, from consumer products to specialised chemical compositions (Büchel, 1985; Halim et al., 2011). In 2020, global chemical-related sales had an estimated value of €3.471 trillion (CEFIC, 2020). However, in recent decades, the negative impacts have become increasingly more apparent; most notably, environmental degradation via increased pollution and resource exploitation, and adverse effects to human health and wellbeing via toxic chemical processes (Anastas & Warner, 1998; Braungart et al., 2007; Rockström, 2009; Halim et al., 2011; Glavic et al., 2021). Therefore, in order to create a more sustainable society, process design must be approached in a holistic way that has not been truly explored before in the literature (Sheldon, 2018), particularly in the context of chemical process plants (CPPs).

The following sections (C.2-.5) of this literature review assessed and discussed CPPs, as well as what is required for a process design to be safe, efficient, resilient, and reliable. This includes safety, overall efficiency, and the potential for sustainability and sustainable development. Moreover, the literature review aided in the design and development of holistically (green and) sustainable MCDM frameworks with WPD philosophy for CPPs, culminating in the systematic integration of PSE tools with MCDM (FAHP-VIKOR and PROMETHEE-II). Such frameworks are further elaborated upon in the project's overall methodology and later chapters.

C.2 Research Questions

- How extensive is the role of safety in CPPs? Does it relate to the efficiency and resilience of the system? How has sustainability been implemented in CPPs, and how can this be linked to the topics discussed in the overall literature review for this project?

- What are typical process design frameworks for CPPs? And how have such frameworks been applied using case studies from the literature?

- How could WPD prove useful within the context of sustainability in CPPs, when compared to a "standard" process design?

C.3 Chemical Process Plants

Process design is an iterative process that consists of MCDM at various steps and stages (Cano-Ruiz & McRae, 1998; Halim et al., 2011). In the context of CPPs, plant process design should involve the development of a multi-dimensional and multi-scale framework for improvement and optimisation, especially when striving towards green(er) sustainability (Halim et al., 2011; Pasman et al., 2020; Di Carlo et al., 2021; Glavic et al., 2021). However, complete process understanding is often time-consuming and too costly to be feasible, especially in the long-term (Sharratt, 2011). Therefore, section C.3 will only discuss the salient areas of plant design based on findings in the literature, to be applied to this project: safety, resilience, overall efficiency, and sustainability.

C.3.1 Safety

Safety is an integral part of the chemical process industry, often in a multi-dimensional approach. This can range from via a socio-economic and/or an environmental dimension, such as using non-toxic solvents in chemical processes to protect the workforce, local/general populaces, and the natural environment (Anastas & Warner, 1998; Patsatzis et al., 2004; Ramzan et al., 2006; Pasman et al., 2020). Major chemical plant-related accidents across the globe, such as the 1976 Seveso explosion and the 1984 Bhopal gas tragedy, have increased public awareness of the potential impacts resulting from such accidents (Patsatzis et al., 2004; Eskenazi et al., 2018; Matilal & Adhikari, 2020). Moreover, the consequences of major chemical accidents have deepened our understanding of how chemical processes can affect human health and the environment, from increased toxicity in human systems to ecosystem degradation (Brown, 1987; Gardea-Torresday et al., 2002; Hall, 2002; Järup, 2003; Braungart et al., 2007; Iravani, 2011; Eskenazi et al., 2018). Therefore, the development of hazard identification, risk analysis (RA), preventative methods, and emergency response initiatives is paramount to the safety component of CPPs (Ramzan et al., 2006; Hosseinnia et al., 2018; Pasman et al., 2020).

In the context of CPPs, safety reviews must be carried out to maintain a certain level of safety (and resilience, section C.3.2), in conjunction with the application of multi-dimensional analysis techniques (Ramzan et al., 2006; Pasman et al., 2020) (Appendix F). Emergency Response Guidelines (ERGs) must also be stringently followed within intentionally-certified management system frameworks, such as those established by the International Standards Organisation (ISO) (Terano et al., 1983; Ramzan et al., 2006; Kotek & Tabas, 2012; Sanders, 2015; Pasman et al., 2020) (Appendix G). Similarly, to MCDM frameworks, RA and hazard identification are overall more effective in a well-structured and optimised management framework, especially when the aforementioned techniques are integrated with each other (Ramzan et al., 2006). Effective CPP management also integrates safety, resilience, overall efficiency, and sustainability (or at least, the capability for sustainability/sustainable development). This can be attributed to the interlinked nature of CPP components, as a well-managed system is more likely to be safer and therefore (more) resilient, and a resilient CPP should theoretically be more sustainable (Pasman et al., 2020; Di Carlo et al., 2021). Therefore, it is essential that CPP decision-makers must approach safety (and the other key aspects of CPPs) in the long-term from a holistic perspective that does not neglect the social dimension (Pasman et al., 2020; Di Carlo et al., 2021; Glavic et al., 2021).

C.3.2 Resilience

In the context of CPPs, resilience can be defined as the ability to maintain or restore reliable operational performance, even after the system has been damaged or disrupted (Dinh et al., 2012; Palazzi et al., 2014; Ganesan & Elamvazuthi, 2017; Pasman et al., 2020). There are twelve main principles to resilience that must be considered for the design of (more) resilient CPPs: failure minimisation, impact mitigation, elasticity/flexibility, early detection, controllability, administrative procedures/controls, safety management, emergency response, human error, design, and potential to detect and/or avoid disruption (Dinh et al., 2012; Pasman et al., 2020). If a CPP is designed without the aforementioned principles in sufficient detail, small incidences can potentially lead to larger, more damaging consequences (Dinh et al., 2012; Palazzi et al., 2014). Resilience is intrinsically linked to safety, efficiency, and sustainability (Palazzi et al., 2014; Moreno-Sader et al., 2019; Pasman et al., 2020); unsafe process designs and work practices can lead to negative holistic impacts, as well as reductions in CPP resilience and overall efficiency (Moreno-Sader et al., 2019; Pasman et al., 2020). Therefore, resilience engineering is a key component of CPP design, that has become increasingly more prominent and prevalent in the literature (Ganesan & Elamvazuthi, 2017; Moreno-Sader et al., 2019; Pasman et al., 2020).

However, the capability and potential to be resilient can be limited by various factors, including holistic factors; for example, maintenance resource availability, mechanical/technical insufficiencies, and the random probability of accidents (Dinh et al., 2012; Ganesan & Elamvazuthi, 2017; Moreno-Sader et al., 2019). Therefore, CPPs must work with and around limitations, which are usually site-specific, in order to become more resilient (Pasman et al., 2020). Furthermore, effective assessments and management of CPPs are crucial towards incorporating and/or improving resilience, in addition to other important aspects; safety, sustainability, and efficiency (Dinh et al., 2012; Moreno-Sader et al., 2019; Pasman et al., 2020). Moreno-Sader et al. (2019) developed a Safety and Sustainability Weighted Return on Investment Metric (SASWROIM) framework integrated with reliability and resilience components, designated as S2R2WROIM. As opposed to the standard return-on-investment (ROI) assessment tools, S2R2WROIM would include resilience (and reliability) into the multi-objective decision-making process, followed by individual metric, process design, and performance analyses. Overall, the novel framework was developed to determine the most viable process design alternative(s), from a holistic perspective; a set of philosophies that can be applied to this project's process design.

C.3.3 Sustainability & Efficiency

Process design is heavily influenced by megatrends, which can influence perceptions, processes, and activities on a long-term scale. Megatrends can form from the impacts of climate change, technological breakthroughs, and socio-demographic changes (Glavic et al., 2021). Initially, sustainability and sustainable development in process design (or "PD&SD") focused primarily on the ecological/environmental aspects (Glavic et al., 2021). However, with increasing awareness of the multi-dimensional nature of sustainability, and the development of more stringent laws and regulations, the incorporation of other criteria—social, economic, and/or political—in PD&SD has become essential towards (holistically) green sustainability (Hopwood et al., 2005; Kerk & Manuel, 2008; Geidoessfer et al., 2017; Glavic et al., 2021). On the other hand, it is rare for PD&SD to be approached via a social dimension, especially in comparison to an economic and/or environmental perspective(s) (Geissdoerfer et al., 2017; Kirchherr et al., 2017). It is clear from sustainability goals, like the UN Sustainability Development Goals (UN-SDGs), that green sustainability—and by extension, CPP efficiency—must be approached holistically, with the implementation of potentially radical changes in (and out of) a CPP context (Morton et al., 2019; Walsh et al., 2020; Cohen et al., 2021; Sarkodie, 2022).

Overall, this will involve a shift in perspective, from the fulfilment of short-term economic goals, to achieving long-term and large-scale green sustainability via (more) energy/resource-efficient systems, such as circular economies (see section A.4) (Kalidindi & Jagirdar, 2012; Wang et al., 2012; Lieder & Rashid, 2016; Glavic et al., 2021). As explained throughout this section, an effective CPP management system framework incorporates sustainability with resilience, efficiency, and safety (Sheldon, 2018; Moreno-Sader et al., 2019; Pasman et al., 2020); this is best exemplified by the use of the S2R2WROIM framework in Moreno-Sader et al. (2019), and the Triple Bottom Line (TBL) framework (Bartelmus, 2013; Geissdoerfer et al., 2017). Therefore, process design for this project must adopt a more holistic philosophy for improving overall efficiency and green sustainability in CPPs. Section C.4 provides an overview of this philosophy, known as Whole Process Design (WPD).

C.4 Whole Process Design

WPD is a process design philosophy introduced by Britest Ltd, that approaches holistic green sustainability design-making, in the context of flexible plant design and chemical processing (Garvare, 2002; Sharratt, 2011; Hodgett, 2016). More specifically, WPD (Figure 2.2) encompasses the entire process design, instead of implementing changes on a step-by-step basis (Sharratt, 2011; Hodgett, 2016). WPD philosophy requires the process designer to identify and understand the characteristics and variables that constitute optimal (and feasible) process design, often with insufficient or incomplete data (Sharratt, 2011; Hodgett, 2016). Moreover, it is imperative that a thorough process understanding is obtained, in order to ensure that decision-making results in a reliable and holistic project methodology (Garvare, 2002; Sharratt, 2011; Hodgett, 2016). Process understanding can be mired with various levels and sources of risk, error, and/or failure; (over-)complexity via unpredictable interactions, insufficient understanding of the system's inner-workings, erroneous understanding of system constituents, and parametric uncertainties that can affect accurate prediction (Sharratt, 2011). Such sources of error/failure can only truly be mitigated—if not resolved—through continuous experimental investigations, that can be costly and time-consuming (Sharratt, 2011; Hodgett, 2016). In fact, it is not uncommon to face greater uncertainties during the early development stages of process design, due to limited or incomplete understanding (Wang & Yang, 2012).

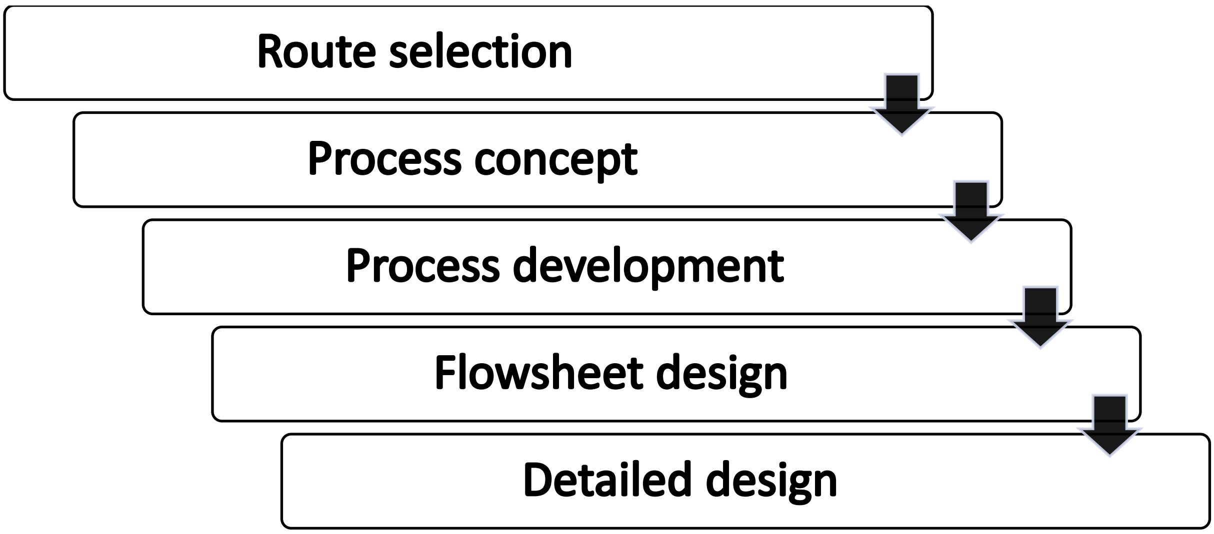


Figure 2.2. A simplified outline of the WPD philosophy by each stage

'Route selection' consists of two main components: the selection of the chemical reactions, and the selection of raw materials. Said selections should be based upon various factors with a holistic mindset, including but not limited to business aims, chemistry manufacturability, and (potential) causes of harm to human health. It is not uncommon for businesses to combine two or more WPD stages, particularly the combination of 'process concept' and 'process development' (Sharratt, 2011). However, it is not recommended to combine WPD stages; instead, each stage should be approached in a (semi-)relaxed stage-gate format (Figure 2.3), in which certain criteria will have to be met to progress onto the next stage(s) (Sethi & Iqbal, 2008; Sharratt, 2011).

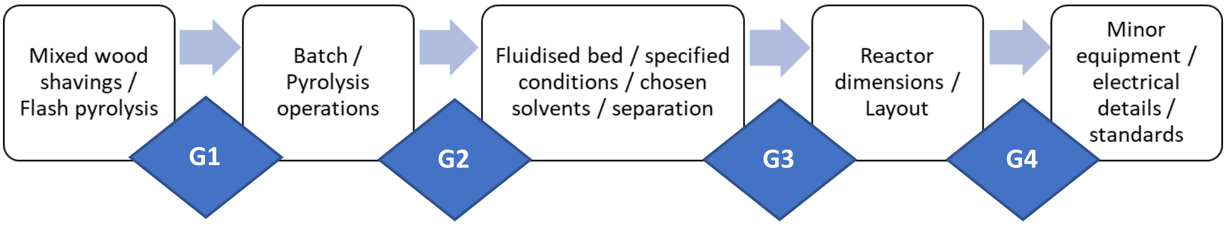


Figure 2.3. WPD philosophy applied to flash pyrolysis; G-*n* represent stage-gates with criteria that must be fulfilled before progression

All reactants should ideally be bought rather than made, for the sake of practicality. Furthermore, to save time and lower overall costs, batch processing was deemed more preferable, albeit this can vary depending on the project. 'Process development' defined the type of equipment that was used for the project. Additionally, this stage had to identify any solvents and separation techniques that were to be utilised. 'Detailed design' was an extension and refinement of 'flowsheet design'. This stage of the WPD involved the identification and implementation of minor equipment, a refinement of the layout in greater detail, and the defining of the electrical and control details.

C.5 Conclusions

Chemical processes are an integral component of modern society, but the negative impacts have also become increasingly more apparent over the years; this includes but is not limited to environmental degradation and adverse effects on human health. Moreover, while previous literature has explored green(er) sustainability in chemical processes, it has never been approached from a truly holistic perspective, particularly in relation to chemical process design for CPPs. CPPs must consider the most essential components, which the literature has identified as (plant) safety, resilience, overall efficiency, and sustainability. Said components are intrinsically linked to each other in process design, i.e., a safer CPP is more likely to be resilient/efficient/sustainable, though this is not guaranteed. This project aimed to develop a truly holistic process design framework for a CPP, albeit complete process understanding was regarded as too time-consuming and costly to be feasible. Additionally, there are (usually) site-specific factors—socially, economically, and/or technically—that can limit the capability and/or potential for the improvement of CPPs. This is further complicated by megatrends in the chemical processing industry, such as in technological breakthroughs and socio-demographic changes which can influence perceptions, activities, and processes at various spatial-temporal scales.

Nevertheless, 'Chemical Process Plants' did provide a solid foundation on CPPs and process design. Said foundation was paramount to the development of novel process design frameworks, by identifying and discussing the key components of CPP design, and the adoption of a WPD philosophy that could lead to significantly greener sustainability in CPPs. To elaborate, the adoption of a WPD philosophy will change how we approach holistically green sustainability in (and out of) CPPs; instead of approaching process design on a step-by-step basis, designers must identify and understand the entire system for the most optimal chemical processes. Although not without its limitations, WPD could present a novel approach towards holistic green sustainability in a CPP context, especially when integrated with PSE tools and MCDM frameworks.

Chapter 3 elaborates on the proposed methodology frameworks, in terms of MCDM and PSE tools, with respect to the key aspects of CPPs that were identified and discussed in sections C.3-.4. Additionally, Chapter 3 explains the steps that were undertaken in the design and proposed implementation of the novel methodology frameworks, from MCDM method(s) to sensitivity analysis.

3. Overall methodology

3.1 Introduction

Chapter 2 is an in-depth literature review into the most relevant key areas of green sustainability: GC, MCDM, and CPPs. Said chapter provided in-depth analyses and discussions into specific GC topics (Appendix D), as well as prominent MCDM methodologies, and the key components of CPPs that must be considered for holistically green sustainability. Moreover, the literature review highlighted the research gaps of previous studies, that ideally should be addressed in the methodology of this project. Most notably, it was determined that the social dimension of green sustainability is often neglected, particularly in comparison to the economic and environmental dimensions (Awasthi et al., 2017; Kirchherr et al., 2017; Mattioda et al., 2020). Furthermore, sensitivity analysis was absent in most of the reviewed literature, which can cast doubts to the overall robustness of certain methodologies (Awasthi et al., 2017; Ali et al., 2019).

The following sections in this chapter outline and explain the design and development of the project's progressively more intricate methodology frameworks across four CPP case studies; three simulation-based (chapters 4-6), and one experiment-based for experimental validation (chapter 8). Said proposed frameworks aim to improve upon each preceding methodology framework. Section 3.2 lists the aims and objectives that were achieved by the project. Section 3.3 explains the project's MCDM methodology, and how it was integrated with the respective methodologies in the aforementioned sections. Lastly, section 3.4 covers the utilisation of Process Systems Engineering (PSE) tools, and their systematic integration with FAHP-VIKOR and PROMETHEE-II to form the final, optimised methodology framework.

3.2 Aim & Objectives

- Aim: Establish the process design using WPD philosophy
  - **Objective 1:** Define the requirements for each WPD stage; i.e. main reactions, raw materials, continuous/batch, layout, and major/minor equipment
  - **Objective 2:** Determine the most suitable set(s) of operation conditions/parameters based on overall feasibility, and the known variables and process interactions
  - **Objective 3:** Run process design simulations via Aspen Plus and/or HYSYS for each of the three simulation-only case studies: sustainable water desalination, IPA synthesis, and green NH_3 production
  - **Objective 4 (if applicable):** Re-evaluate the most appropriate criteria (and sub-criteria) for the MCDM framework

3.3 MCDM framework

3.3.1 Method selection

The literature review has analysed and discussed the extensive history of its applications in various disciplines, from local Amazon book sales (Bandyopadhyay, 2020) to urban sewer network planning (Wu & Abdul-Nour, 2020). In the context of green sustainability and sustainable development, MCDM frameworks—individual and/or integrated—have significant potential for holistic applications in CPPs (Fonseca et al., 2021; Kannan et al., 2021). Each MCDM method has their respective strengths and limitations, which are summarised in Table 3.1. Therefore, it is imperative that we choose the most suitable MCDM methods, to develop into an MCDM framework for the project. Based on our findings from the literature review, MCDM hybridisation is highly recommended, if not essential, towards a more equally holistic approach than ever before (Behzadian et al., 2010; Stojcic et al., 2019; Jamwal et al., 2021). Additionally, hybridised "integrated" MCDM frameworks optimise the decision-making process and mitigates/resolves the limitations of an individual MCDM method.

The project involved the design and implement several Posteriori MCDM frameworks of progressively greater intricacy: FAHP, FAHP-TOPSIS, and FAHP-VIKOR with PROMETHEE-

II, and PSE tools with FAHP-VIKOR & PROMETHEE-II. "Fuzzy" logic was incorporated into AHP to reduce the input uncertainty and enable more consistent, more representative rankings (Awasthi et al., 2017; Vakilipour et al., 2021). Pre-selected groups of decision-makers—professionals and experts in various sustainability-related research fields—used FAHP to weigh criteria and sub-criteria, as well as evaluate the criteria with linguistic qualitative assessments that were converted into TFNs. TOPSIS, VIKOR, and PROMETHEE-II were implemented to rank the potential pathways of each case study, before sensitivity analysis was then applied to evaluate the overall robustness of the proposed frameworks. Sections 3.3.2-.3.4 go into further detail on the MCDM methodology, such as how MCDM was integrated into the project's proposed overall methodology.

Table 3.1. The strengths, limitations, and recommended software aid for the most prominent MCDM methods in the literature

MCDM	Recommended software (*Optional)	Strengths	Limitations
(F)AHP	None; *Excel	Highly flexibility & adaptability Simple and easy to use; arguably, the most commonly used MCDM (with fuzzy logic) in the literature Does not involve a complex algorithm; possible manual incorporation Clear hierarchical structure; criteria (and sub-criteria) are transparent and given focus	Interdependency among alternatives and objectives Data must be derived from experience Unequal focus on criteria/sub-criteria (i.e. their weightings) via participants, particularly involving qualitative data
VIKOR	Excel; MATLAB	Compromise solution is derived from quantitative and qualitative data; therefore, a more accurate and reliable representation of decision-maker viewpoint(s) Ideal MCDM for situations where target objectives cannot be fully conveyed, e.g. supplier selection Linear normalisation removes criterion units;	Relative instability; conflicts can lead to changing rankings, such as rank reversal Developing a reliable real-time model can be time-consuming and difficult to implement, particularly with quantitative data

		normalised values are independent of criterion evaluation unit	
TOPSIS	None; *Excel; *Python; *MATLAB	Does not involve a complex algorithm; possible manual incorporation Independent criteria are not required	Vector normalisation is required for multi-dimensional problems; this can alter criteria data Euclidean distance between ideal solutions is not properly considered; optimum alternative may not relate to closeness to the ideal solution Use of crisp data values requires fuzzy TOPSIS for full effectiveness and reliability
ELECTRE-III	ChemDecide	Can handle discrete, heterogeneous criteria (qualitative and quantitative) Can accept or avoid trade-off (i.e. compensation), though this depends on the decision-makers Unlike AHP, alternative comparisons can be derived, even without specified preferences Ideal for situations involving strong sustainability and energy planning ChemDecide enables decision-makers to apply a greater number of criteria, compared to simpler MCDM methods	Cannot be easily summarised into a step-by-step process Avoiding compensation involves knowing and understanding specialised knowledge of the objectives Not intuitive to use; ChemDecide can mitigate the issue, but decision-makers must know how to use it/them Rank reversal can still be an issue, when handling a high number of criteria/sub-criteria
PROMETHEE-II	*Excel; Smart Picker Pro; D-sight; Visual Promethee	Decision-making is a collaborative process Ranking consistency, due to using “true” (non-	Comparatively less versatile Potentially less reliable at

		normalised) qualitative and quantitative data Provides conclusive optimal alternative(s), compared to ELECTRE Data does not require normalisation, unlike TOPSIS or ELECTRE Unlike ELECTRE or TOPSIS, gray data, i.e. insufficient/missing data, can be used	producing conclusive results Criteria may not be fairly weighted by decision-makers, particularly with a high number of criteria Without software aid, algorithm complexity can lead to a time-consuming MCDM process Smart Picker Pro: free trial has unlimited use, but limited no. of criteria

3.3.2 Equipment & tools

Because FAHP does not involve complex algorithms (section B.3); it was manually implemented with relative ease. For the sake of time and resource accessibility, the following software platforms were utilised in this project: Excel (FAHP and FAHP-VIKOR with PROMETHEE-II) and MATLAB (FAHP-TOPSIS only). Ideally, Table 3.1 illustrates that VIKOR and PROMETHEE-II should have been employed via MATLAB and Smart Picker Pro (Wu & Abdul-Nour, 2020), respectively. That being said, Smart Picker Pro would have likely required a considerable degree of training for decision-makers, and usable MATLAB code for VIKOR was unavailable at the time.

3.3.3 Selecting & weighting criteria/sub-criteria

Table 3.2 outlines the hypothetical "unrefined" sustainability-related sub-criteria for each criterion that this project had identified via the literature review, prior to the establishment of case-specific sub-criteria. Specialised software platforms, such as Aspen Plus v12 and SimaPro v9.6.0.1, were used to determine the relative significance (i.e. impact) of individual criterion and sub-criterion via process simulation. The three most significant sub-criteria per criteria/dimension were subsequently identified, weighted, and then tabulated via FAHP and the Delphi method (i.e., structured communication among decision-makers). Since the number of criteria and sub-criteria cannot be too large without becoming too costly and time-consuming, this was deemed as a sufficient number of sub-criteria per criteria. Every other sub-criteria was discarded, due to not passing the threshold in terms of significant impact, especially those of negligible value. Additionally, to avoid potential "decision fatigue" and stay focused, decision-makers were instructed to take mandatory breaks at regular intervals.

Criteria and sub-criteria weighting were carried out via pairwise comparisons, with respect to the established aims and objectives of the project (section 1.1). The pairwise comparisons had used qualitative linguistic assessments relative to a 6-point scale; 1=equally important, 3 or 1/3=Moderately (more/less) important, 5 or 1/5=Significantly more/less important, to be converted into TFNs. Because (F)AHP data aggregation could have resulted in inaccurate representative consensus among decision-makers (Cheng, 2004), the combined coefficient *u* was set to 0.5, where appropriate to minimise potential information loss. However, for the pathways to be ranked via TOPSIS/VIKOR and PROMETHEE-II, the TFNs had to be further processed into crisp numerical values with Eq.1.

Table 3.2. Hypothetical sub-criteria per criterion. Process simulation in Aspen Plus/HYSYS v12.0 was implemented, to define the most significant sub-criteria from the weightings specific for each case study

Criteria	**Social**	**Environmental**	**Economic**	**Technical**	**Safety**
Sub-criteria	Design; based on location-specific demands/requirements	Global warming potential	Yield factor	Tech maturity	Chemical exposure
	Policy applicability	Fuel consumption	Raw material costs	(Overall) feasibility	Fire hazard risk
	Energy security (effects)	Raw material consumption	Water costs	(Overall) capability	Chronic toxicity risk
	Social acceptability	Waste yields		Green performance	

3.3.4 Most optimal pathway(s)

Each framework aimed to be validated via determining the most optimal pathway in small-scale case studies based on rankings via criteria and sub-criteria weightings. Qualitative data (i.e., non-numerical) data was converted into TFNs and subsequently into crisp numerical values for MCDM applications. Section B.3 outlines (F)AHP, while section B.6 explains the VIKOR methodology, in which rankings were based on the Q_i values. A step-by-step summarisation of alternative ranking via PROMETHEE-II is provided in section B.7, in which rankings was based upon net outranking flows, φ or $\varphi(a)$. Additionally, sensitivity analysis was applied to evaluate the robustness of each MCDM framework. If it had been applicable, rankings were amendable, albeit not without a series of collaborative discussions among decision-makers. Figure 3.1 summaries the first-draft (I) and final, optimised (II) versions of the proposed methodology framework.

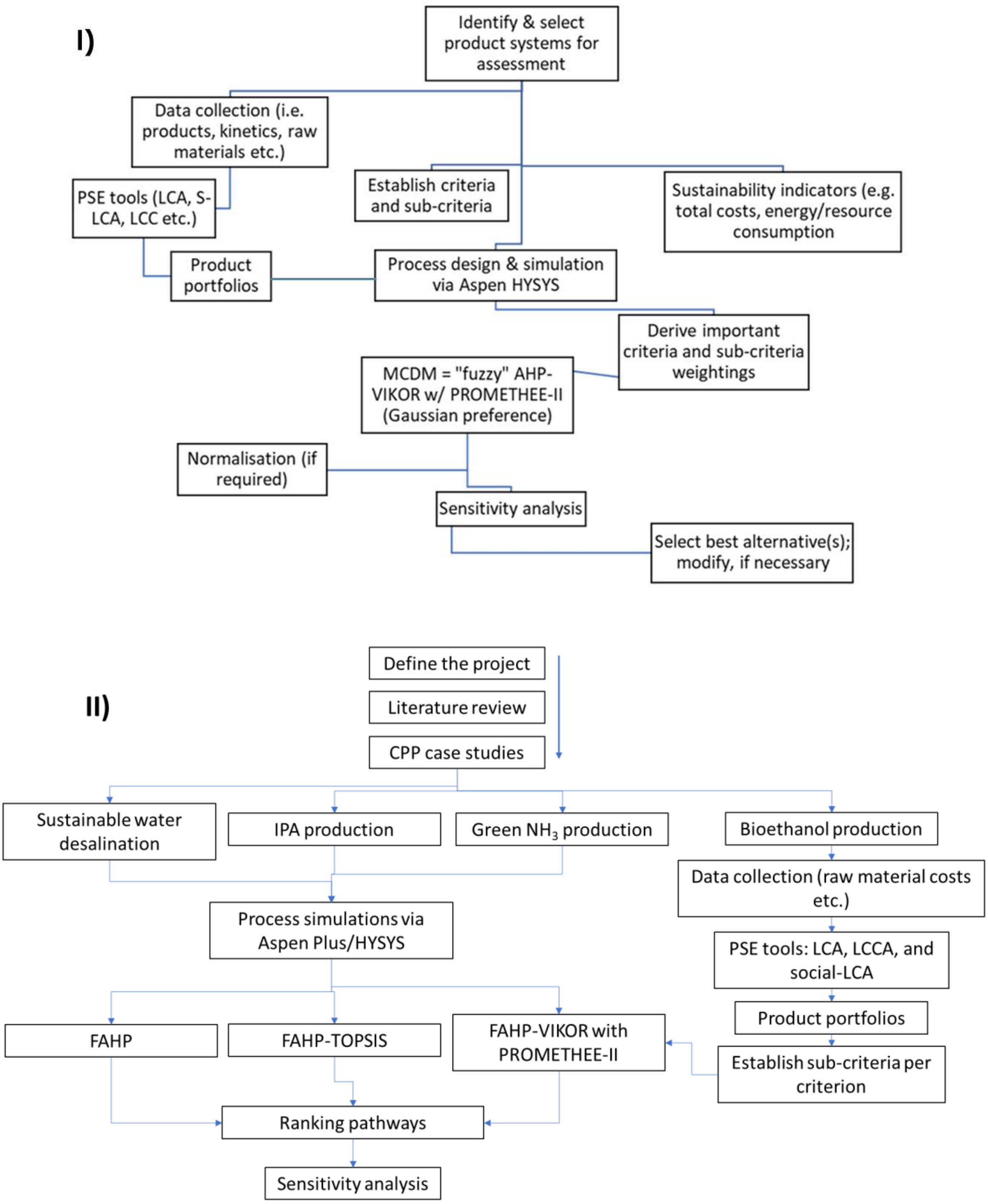


Figure 3.1. Proposed top-to-bottom methodology framework for the project, I) First draft; II) Final, optimised version. Order of methodology steps in (II) is denoted by the arrow directions

Both (I) and (II) have the same overall steps: system (i.e. case study) identification→data collection, process simulation, and defining key sustainability criteria/sub-criteria→MCDM→sensitivity analysis. (II) was the optimised result of (I), with a more clearly defined structure. Specifically, in the following order of steps/stages: defining the project and using literature review to establish the four representative cases, process simulation via the

Aspen Plus/HYSYS v12, MCDM via the methodologies in Figure 3.1 to prioritise pathways, and sensitivity analyses to evaluate the overall robustness. PSE tools were systematically integrated with MCDM (FAHP-VIKOR with PROMETHEE-II only), to establish the key sustainability sub-criteria for the bioethanol production, in contrast to the three simulation-based case studies.

3.4 Process Systems Engineering (PSE) tools

PSE tools have been extensively implemented throughout various research fields, particularly in (green) sustainability (Ren et al., 2015; Mattioda et al., 2020; Rebolledo-Leiva et al., 2023). The most prevalent PSE tools are LCA and LCCA for the environmental and (techno-economic dimensions of sustainability (Goedkoop et al., 2016; Bhonsle et al., 2022), albeit social-LCA is becoming increasingly more prevalent in implementation (Mattioda et al., 2020; Bouillass et al., 2021). However, social-LCA is underdeveloped and thus not/rarely fully utilised, largely due to the underdeveloped and/or lack of social databases (Valente et al., 2018). This is particularly evident in comparison to LCA and LCCA (Mattioda et al., 2020; Srinophakun & Suwajittanont, 2022). The final stage of the project aims to validate and further expand upon the works of Ren et al. (2015), in regard to an experiment-based validation case study: bioethanol production (chapter 8). Specifically, the development and employment of a holistically green sustainability governance platform via the systematic integration of LCA, LCCA, and social-LCA with a more robust and stable MCDM framework (FAHP-VIKOR & PROMETHEE-II). Section 8.6 provides further details on the required steps for LCA, LCCA, and social-LCA: goals & scope, functional unit(s), system boundaries, and inventory analysis.

3.5 Conclusions

Several "fuzzy" MCDM frameworks have been proposed, with each of the following more intricate than the last: FAHP, FAHP-TOPSIS, and FAHP-VIKOR with PROMETHEE-II, and PSE tools with FAHP-VIKOR & PROMETHEE-II (chapters 7-8). The project's final, optimised methodology framework implemented a truly holistic approach towards green sustainability in small-scale, modular CPPs. Specifically, the systematic integration of FAHP-VIKOR & PROMETHEE-II framework with PSE tools (LCA, LCCA, and social-LCA) under a WPD philosophy. The integrated MCDM frameworks were developed to address the limitations associated with each individual MCDM methodology. Ideally, if they had been available, specialised software platforms and/or packages should have been utilised for the implementation of certain MCDM methodologies and PSE tools; SimaPro for the PSE tools, MATLAB for VIKOR, and Smart Picker Pro for PROMETHEE-II. Moreover, sensitivity analysis was employed to evaluate the robustness of the aforementioned methods. The project proposed an overall methodology that utilised MCDM, WPD philosophy, and PSE tools to be more holistically green and/or sustainable than previous sustainability-related works, especially in the context of CPPs. Four small-scale, modular CPP case studies (chapters 4-6,8) have been chosen to validate the project's methodology.

4. Sustainable water desalination in Oman

4.1 Overview

As the global human population continues to grow and become increasingly more urbanised, groundwater and surface water resources are close to becoming/have become outpaced by demand in many regions (Nair and Kumar, 2013; Loutatidou et al., 2017; Mahmoudi et al., 2023). Presently, over 780 million people globally do not have (easy) access to clean, safe drinking water (UN, 2022; Mahmoudi et al., 2023). This can have severely negative impacts upon the holistic development of a country/region, in areas such as (but not limited to) economic growth, education, infrastructure, social justice, and responsible resource consumption/utilisation (Gude, 2016; Loutatidou et al., 2017). The oceans (~97% of the planet's available water) could be the key towards addressing water scarcity, but only if the high salinity is addressed (i.e. the brine is extracted). Water desalination is a process in which brine is extracted from seawater/brackish, therefore deriving freshwater that can also be utilised for various other purposes, such as agriculture (Loutatidou et al., 2017; Mahmoudi et al., 2023).

Approximately half of all conventional desalination units in the world (totalling at >15,000, with a total daily freshwater production rate of ~70 million m^3) are in the Middle East, largely due to being one of the most water-scarce regions in the world (Belessiotis et al., 2016; Loutatidou et al., 2017; Mahmoudi et al., 2023). Thermal and electrical separation are the primary industrial methods for water desalination. High temperature steam vaporises the water, leaving behind the brine (and waste), in the former. In contrast, the latter involves utilising high pressure generated via pressurised water sent through series of membranes (Panagopoulos et al., 2019). Reverse osmosis (RO), an electrical-based technology, dominates the desalination market, with ≥60% of desalination plants using RO (Loutatidou et al., 2017; Panagopoulos et al., 2019). However, in comparison to groundwater pumping, using RO to derive desalinated water is far more costly at USD$0.49-2.89 per m^3 (Voutchkov, 2019).

The key issues associated with desalination are energy costs and the disposal of brine waste. According to the IEA, desalination accounted for 5% of the Middle East's total energy consumption in 2016, while only generating 3% of the region's water supply (IEA, 2019). Figure 4.1 illustrates that ~41% of total costs can be attributed to the energy demands required to generate the necessary temperatures and pressures for desalination, which can also have severe adverse environmental effects (Okampo and Nwulu, 2021). A total of 200 kWh/day is consumed globally by desalination plants, with a ratio of 3-10 kWh to 1 m^3 of desalinated water (<1 kWh for conventional drinking water) (Bienkowski, 2015; Okampo and Nwulu, 2021). Up to 99% of the total energy demand is derived via fossil-fuels (Do Thi et al., 2021).

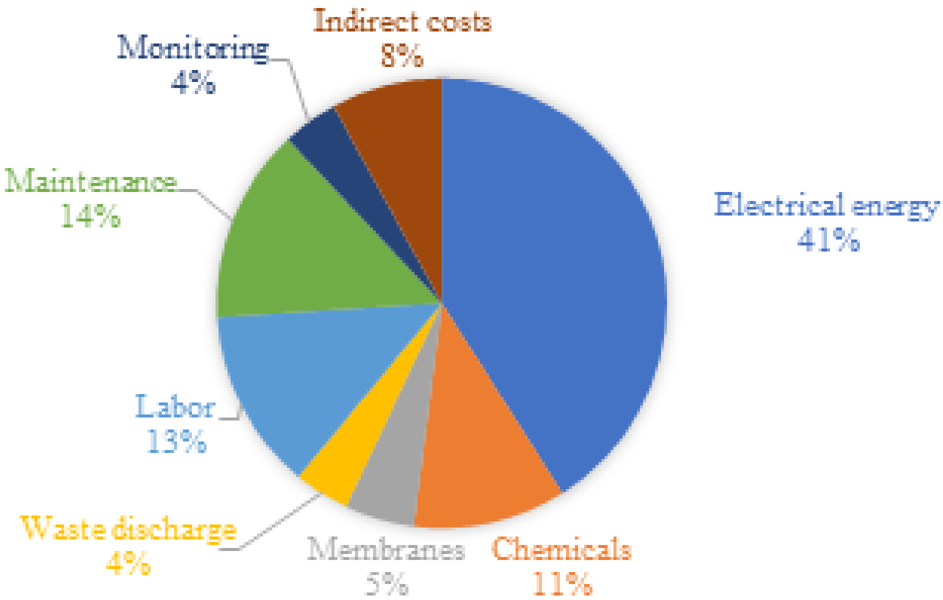


Figure 4.1. Desalination cost breakdown by % (Okampo and Nwulu, 2021)

Desalination plants must therefore transition towards (green) sustainability, which could be achieved with process intensification and modularisation using stranded renewable energy sources, such as wind and solar (Kyriakarakos and Papadakis, 2021). Smaller, modularised plants are overall more cost-effective than downsizing existing large-capacity plants, especially in conjunction with process intensification (i.e. improvements in overall efficiency, reduced overall costs, and better water quality). RO systems are optimised towards smaller, modularised plants, as they have an adaptable and easily maintainable modular membrane design, albeit this requires further design development (Kyriakarakos and Papadakis, 2021). That said, said systems are highly geared towards process intensification for various additional reasons, especially due to developments in recent decades: low energy intensity, high efficiency, low capital costs, and high selectivity/permeability regarding transportation components (Drioli et al., 2017).

MCDM could be the key towards incorporating and/or enhancing the sustainability of small-scale desalination process for rural populations via the selection of the most optimal potential pathway(s), based on (green and) sustainable criteria. Section 4.2-.5 details a case study regarding a relatively small-scale (i.e. community-scale) RO desalination and water treatment plant system in Sohar, Oman. Moreover, section 7.2 elaborates on the validity of a FAHP framework to rank the desalination pathway(s) via MCDM, based on sustainability criteria.

4.2 Modelling

The standard plant configuration is single-pass RO with continuous operation. Improved recovery was achieved via small-unit recirculation of reject water, albeit this was not modelled in the case study. Desalination process design and modelling insights were obtained from Zaidi and Saleem (2021). Whenever and wherever possible, water sample information was acquired from numerous sources for the Gulf of Oman. If this was not possible, the Persian Gulf served as an appropriate substitute, due to its relative proximity. Appendix H lists the model water (Appendix H-I) and design (Appendix H-II) parameters for RO systems, Omani drinking water quality standards (Appendix H-III), and the recommended ion concentrations (Appendix H-IV) for conventional desalination via surface seawater (Sana et al., 2005; Feroz et al., 2012; Joy et al., 2021). The model design has accounted for seasonal-based variations, particularly the maximum range values, in water characteristics and their effects on RO systems (Feroz et al., 2012). Smaller units can improve recovery via the recirculation of reject water, but this was not modelled.

Water flux, the most essential design characteristic, is dependent upon the source(s) and quality of feed water, which in turn affect the risk of membrane fouling (Feroz et al., 2012; She et al., 2016; Jiang et al., 2017; Goh et al., 2018). Therefore, membrane characteristics must be designed to address fouling, for the sake of reliable, long-term (membrane) performance and integrity in sustainable desalination (Jiang et al., 2017; Goh et al., 2018). Water Application Value Engine (WAVE) and Desalination Economic Evaluation Program (DEEP) software were optimised to assess relatively small-scale desalination plants, with an assumed 24 hrs/day operation (daily rates) for modelling consistency. Additionally, model plant life was set to 20 years, with an annual availability of 90% based on the literature findings (Feroz et al., 2012; Jiang et al., 2017; Goh et al., 2018; Zaidi and Saleem, 2021).

4.2.1 Water Application Value Engine (WAVE)

WAVE, developed by Dupont Water Solutions, is a popular software platform for modelling advanced desalination and water treatment technologies (Toth, 2020; Dupont Water Solutions, 2022; Ruiz-Garcia et al., 2023; Luong et al., 2023). Four cases were optimised in Table 4.1 (Bartram et al., 2023): 50, 200, 500, and 1000 m^3/day, with the full parameter details listed in Appendix I (I-I to I-IV, respectively). These four cases were selected to highlight the potential for modular, small-scale design that promotes (green) sustainability, especially in the reduction of overall energy consumption. Moreover, only four cases were analysed and assessed to prevent: 1) an arduous, time-consuming process of designing and modelling several potential pathways over a large range of possible permeate flows, which would have been further exacerbated during the MCDM steps; 2) a detraction of focus from the other cases, which implemented far more intricate methodology frameworks.

Table 4.1. Optimised RO WAVE modelling configurations. Conservative flux rates with acceptable industrial ranges for no. of stages, pressure vessels (per stage), and membrane elements (Bartram et al., 2023)

Parameter	Case A	Case B	Case C	Case D
Permeate flow (m^3/day)	50	200	500	1000
Feed flow (m^3/day)	66.4	265.4	663.6	1327
Pressure vessels	2	4	7	8
No. of stages	1	1	1	2
Membrane elements	2	4	6	5
Mean flux (GFD)	7.5	7.5	7.1	7.5

A conservative-to-typical flux rate range of 7-8.6 GFD was selected, while total energy use (kWh/m^3 of product water) and USD$ price were minimised via adjustments to the following characteristics: pressure vessels per stage, membrane type, number of membrane stages, and membrane elements per pressure vessel. Figure 4.2 shows the typical detailed design for an RO train (Rodriguez-Calvo, 2015).

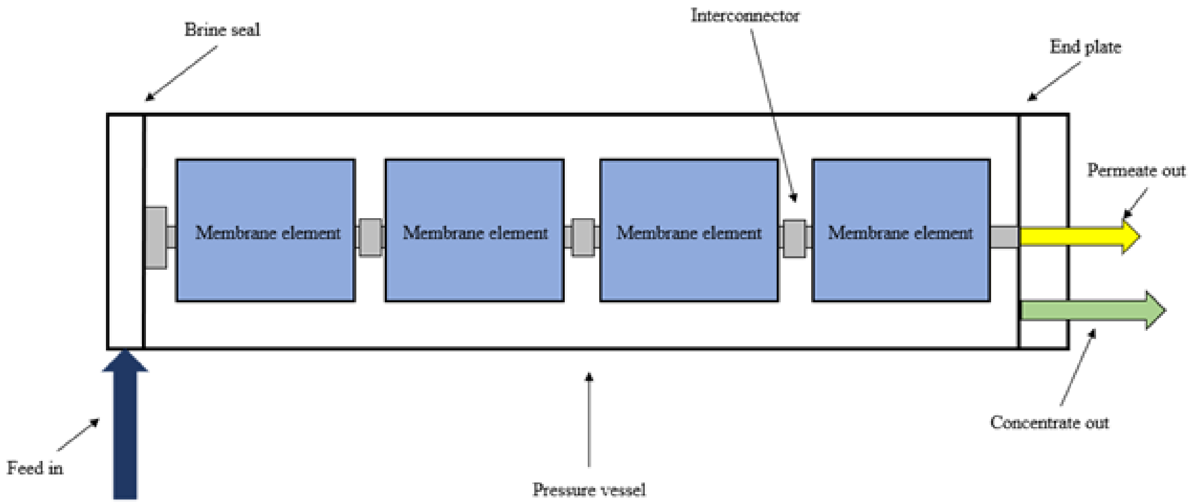


Figure 4.2. Detailed design for a conservative-to-typical RO train (Rodriguez-Calvo, 2015)

WAVE defaults for operating costs were selected (0.14 USD/m^3 and 0.69 USD/m^3), while electricity costs were adjusted to values in Oman, circa September 2022 (Global Petrol Prices, 2022). Each case has an assumed recovery of 75.4% that was used to calculate the input flow rates. Figure 4.3 shows the configuration for Case A, with B-D in Appendix J (J-I to J-III, respectively).

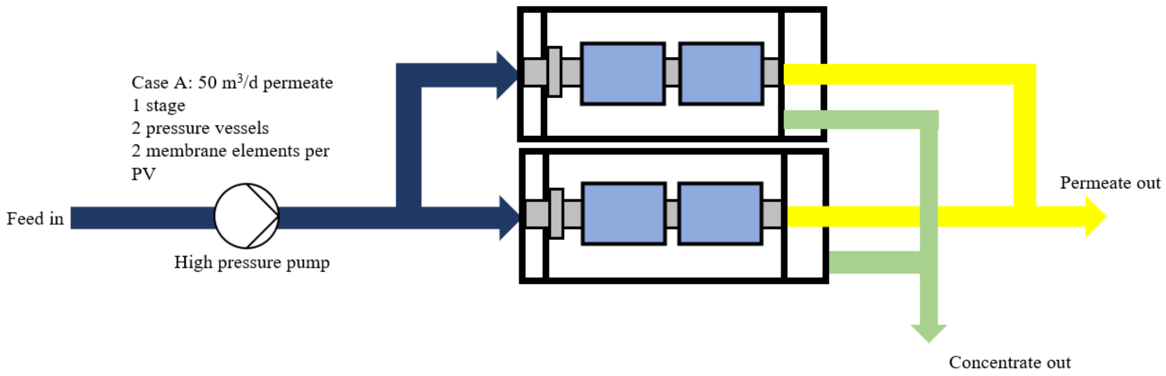


Figure 4.3. RO configuration for Case A (Bartram et al., 2023)

WAVE enabled process design down to the specific, flux-based membrane elements, and water treatment by ion type. Furthermore, the software included economic costs, such as specific water/energy cost(s), albeit it was not able easily ascertain the specifics behind said costs, nor evaluate certain energy sources like renewables and standalone generators.

A Thin Film Composite (TFC) membrane, FilmTec^{TM} SeaMaxx^{TM} 440 was modelled, produced by Dupont Water Solutions (Dupont Water Solutions, 2024), due to having the overall best performance of all WAVE membrane types. Moreover, it was the most suitable choice with respect to moderate temperature and salinity conditions for seawater, as well as its ability to process higher flowrates than its cellulose-based counterparts. That said, future studies should seek to expand the available membrane types for more holistic analyses.

4.2.2 Desalination Economic Evaluation Program (DEEP)

In contrast to WAVE, DEEP is a relatively more complex desalination modelling software that utilises Excel, developed by the International Atomic Energy Agency (IAEA) to highlight the potential of nuclear-powered desalination. That said, unlike WAVE, DEEP is unable to account for individual membrane design. However, it is capable of modelling various electrical- and thermal-based desalination designs that run on alternative energy sources, including but not limited to renewables and/or nuclear power. DEEP can also generate high(er)-level economic information (and sensitivity analysis) via changes in input data; salinity, energy type(s), and plant capacity. More specifically, DEEP can calculate annual capitalised costs via multiplying specific costs by the following factors: in-/outfall, discount rate, owner, contingency factors, interest, and construction lead time. Figure 4.4 summarises the economic evaluation capabilities and methodology of DEEP (Rahimi et al., 2021).

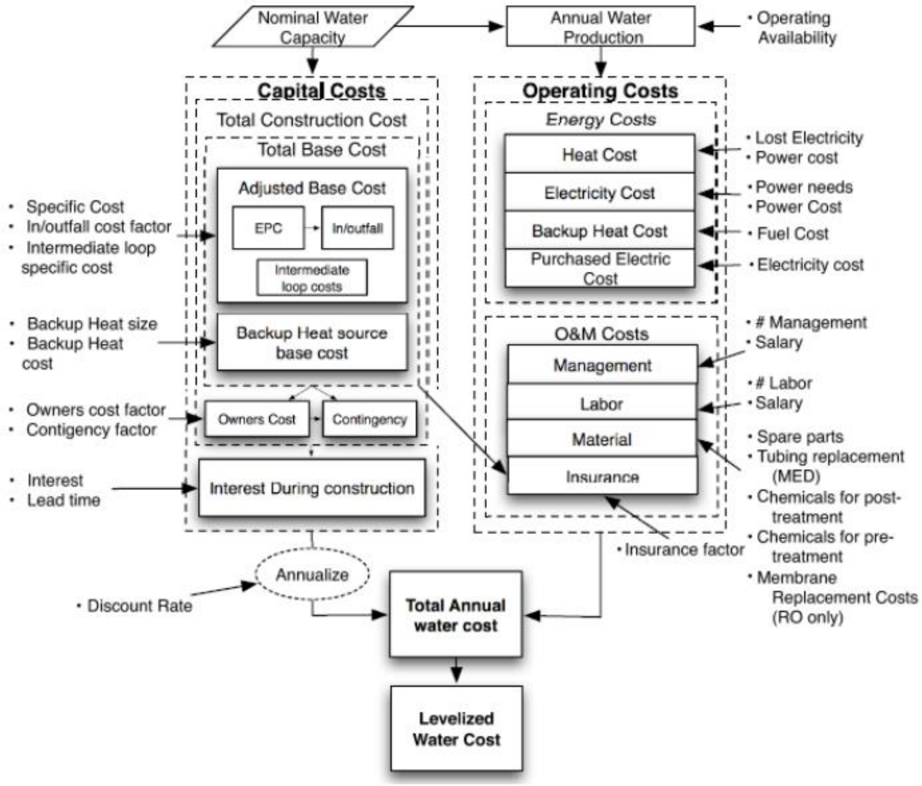


Figure 4.4. DEEP economic analysis flowsheet, DEEP 5 user manual (Rahimi et al., 2021)

Although DEEP has energy options for grid-connected renewables, they were not intuitive to model. Instead, the power type was set to combined cycle gas, without the utilisation of financial data (e.g. operating costs) via the outputs. Therefore, while DEEP proved useful in generating results to cross-compare operating and specific water costs, economic analysis was somewhat less useful for small-scale comparison studies of dedicatedly renewable-powered vs standard generator/grid-powered desalination plants.

4.2.3 WAVE and DEEP results

Specific water costs (in USD/m^3) were generated via WAVE and DEEP simulations, as well as techno-economic analysis literature (Moser et al., 2015; Kettani and Bandelier, 2020), to represent the operating expenses (including electricity costs) and operating (OPEX) & capital expenditures (CAPEX), respectively. Using the cost parameters established by Kettani and Bandelier (2020), CAPEX values for Cases A-D were as followed, in USD: 61,000, 244,000, 610,000, and 1,220,000 (Appendices K-I and K-II). Specific electricity costs (Appendix K-III) were calculated via Wolfram Mathematica and MATLAB code (Appendix L) and WAVE-derived specific energy outputs via Silfab Solar Prime series SIL-370-HC PV panels, when applicable. Appendices M-I and M-II lists the total capital costs and specific energy outputs, respectively, for the desalination plant configurations of Cases A-D, with an assumed 20-year plant life. Total costs were derived via the multiplication of each OPEX/CAPEX parameter by the capacity of each case. Moreover, WAVE produced the water treatment parameters and specific energy cost (in kWh/m^3). However, there were some operating cost inconsistences using DEEP, to the extent that more emphasis was placed upon WAVE's economic analysis for Cases A-D (Table 4.1). For the sake of relative simplicity regarding remote-system operations, Cases A-D represent single-pass systems without recycle elements.

WAVE calculated a water recovery rate of 75.3% in the permeate flow, which indicates an incredibly high level of performance, compared to typical RO industrial standards of 50-85% (Indika et al., 2021). That said, it should be noted that the recovery rate is independent of the other variables, such as adjustments to the specific flow rate of permeate via membrane transport equations. As plant capacity increases, it is generally expected for the specific energy and water costs to fall, due to the latter being a function of water product quantity. However, this trend is far more evident among larger, dissimilar capacities (e.g. >1000-100,000 m^3/day). Table 4.2 illustrates the specific costs produced via WAVE and DEEP, with a complete case-by-case representation relative to plant capacity in Appendices N-I and N-II, respectively.

Table 4.2. Optimised WAVE and DEEP specific costs. DEEP highlights the general trend of decreasing specific costs with increasing capacity, unlike WAVE, likely due to calculation methodologies (Bartram et al., 2023)

Parameter	Case A	Case B	Case C	Case D
Capacity (m^3/day)	50	200	500	1000
WAVE specific water cost (USD/m^3)	1.023	1.147	1.138	1.141
DEEP specific water cost (USD/m^3)	10.67	3.29	1.99	1.5
Specific energy (kWh/m^3)	4.78	5.57	5.52	5.53

Specific operating costs were utilised in the FAHP framework in section 7.2, along with the calculated net present costs for each energy configuration (Figures 4.5-.6). That said, it should be noted that DEEP may overweight labour and management (L&M) costs (Appendix O). This could explain the trend discrepancy between the specific costs and capacities, as L&M costs constitute a large majority of specific costs for smaller plants. Additionally, DEEP is optimised towards (much) larger scale desalination.

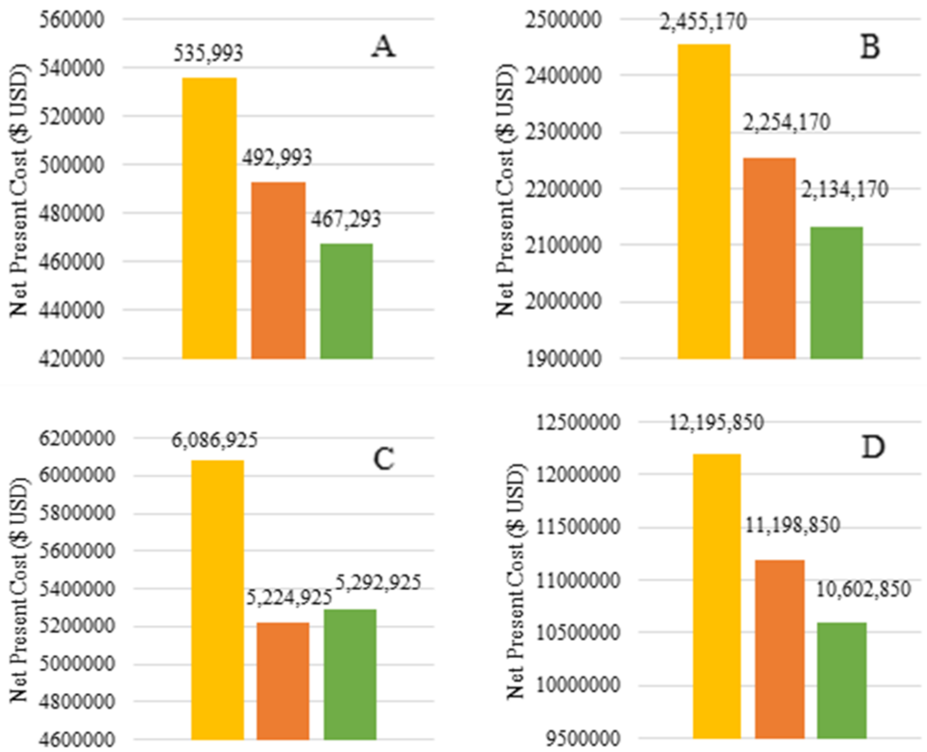


Figure 4.5. Net present, capacity-based costs (Bartram et al., 2023)

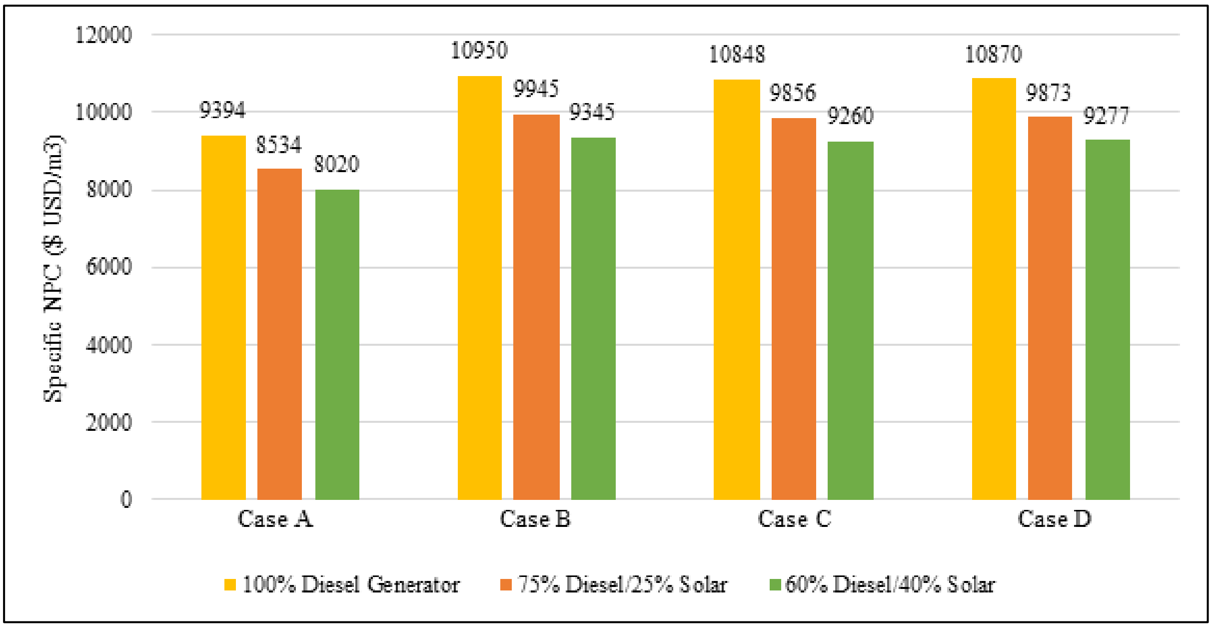


Figure 4.6. Net present costs for energy systems only (Bartram et al., 2023)

Consequently, L&M costs are significantly inflated to scale. Therefore, it is imperative that OPEX is appropriately weighted relative to capacity for economic analysis, to avoid generating abnormally cost-to-capacity disparities via software like DEEP.

4.3 Environmental analysis

In terms of water quality standards, Table 4.3 shows the case-by-case WAVE results for each water quality parameter within the standard range of percentages (~95-99%) for rejected total dissolved solids (TDS).

Table 4.3 WAVE water quality parameters and %TDS (Bartram et al., 2023)

Parameter	Case A	Case B	Case C	Case D
Feed TDS (mg/L)	41,227	41,255	41,253	41,253
Permeate TDS (mg/L)	945	1105	1152	1090
Removed solids (%)	97.7	97.3	97.2	97.4

Sustainable desalination plant design must strive towards reducing energy use and CO_2 emissions. For the sake of simplicity, this section excludes emissions via fuel transportation, solar power system land use, and material life cycles. However, further studies may consider the above emission contributors, for a more holistic environmental analysis. In terms of specific energy consumption, industrial-scale seawater RO desalination plants can reach up to 3-6 kWh/m^3 (Do Thi et al., 2021), as illustrated in Table 4.2 for Cases A-D. There is no strong evidence to suggest an inverse relationship between specific energy consumption and plant capacity. In fact, the specific energy consumption for case A (50 m^3/day) could imply that small-scale configurations are the key to minimising energy use, especially applying intensified plant design. Contrastingly, according to WAVE, the energy configurations did not influence variations in specific energy consumption, since grid energy was considered and not the exact energy configurations listed in Tables 4.4-.5. Table 4.4 highlights the impacts of fuel (usage and cost) on desalination, which can be significantly reduced with solar hybridisation. On the other hand, more solar-leaning hybrid configurations are associated with high upfront capital cost.

Table 4.4. Total OPEX and fuel-related data per energy configuration and case. The energy configurations were calculated in Mathematica (Bartram et al., 2023)

Case	Energy Configuration	Fuel Usage (L/year)	Specific Fuel Usage (L fuel/m^3 water)	Fuel Cost ($ USD /year)	Total OPEX ($ USD /year)
A	100% Diesel	34,890	1.91	21,670	23,410
	75% Diesel, 25% Solar	21,670	1.43	16,250	20,820
	60% Diesel, 40% Solar	20,940	1.14	13,000	19,270
B	100% Diesel	162,700	2.23	101,000	109,100
	75% Diesel, 25% Solar	122,000	1.67	75,760	97,080
	60% Diesel, 40% Solar	97,950	1.33	60,610	89,840
C	100% Diesel	403,000	2.20	250,200	270,400
	75% Diesel, 25% Solar	302,200	1.66	187,700	240,500
	60% Diesel, 40% Solar	241,800	1.32	150,100	222,600
D	100% Diesel	807,300	2.21	501,300	541,700
	75% Diesel, 25% Solar	605,500	1.66	376,000	481,800

	60% Diesel, 40% Solar	484,400	1.33	300,800	445,900

Table 4.5 shows the generated emissions via each energy configuration per case. Fuel usage emissions via the diesel generators were calculated under the assumption that 19.76 g of CO_2 was released per 1 L of combusted fuel (Rezk et al., 2021). The diesel-solar hybrid configurations demonstrated a proportional reduction in emissions to the %utilisation of solar power. That said, such reduction is overstated by the assumption that the diesel generator is responsible for all emissions, when other factors must be considered; namely, PV panel installation life cycle, maintenance, and recycling. Nevertheless, the CO_2 emissions should be considered as reasonable, in terms of the scale of operations. Large-scale operations should expect a specific emissions range of 0.4-0.67 kg CO_2eq/m^3 water (Tal, 2018). Small(er)-scale desalination plants therefore seem to environmentally benefit from modular and intensified designs, relating to the reduction in specific CO_2 (or equivalent) emissions per m^3 of water per year (Figure 4.7).

Table 4.5. Emissions data for each energy configuration per case (Bartram et al., 2023)

Case	Energy Configuration	Total Emissions (tonnes CO_2/year)	Specific Emissions (kg CO_2/m^3 water)	Emission Reduction %
A	100% Diesel	0.69	0.037	-
	75% Diesel, 25% Solar	0.43	0.023	25.0%
	60% Diesel, 40% Solar	0.41	0.023	40.0%
B	100% Diesel	3.21	0.176	-
	75% Diesel, 25% Solar	2.41	0.132	25.0%
	60% Diesel, 40% Solar	1.93	0.106	40.0%
C	100% Diesel	7.96	0.436	-
	75% Diesel, 25% Solar	5.97	0.327	25.0%
	60% Diesel, 40% Solar	4.78	0.262	40.0%
D	100% Diesel	15.95	0.874	-
	75% Diesel, 25% Solar	11.96	0.656	25.0%

	60% Diesel, 40% Solar	9.57	0.524	40.0%

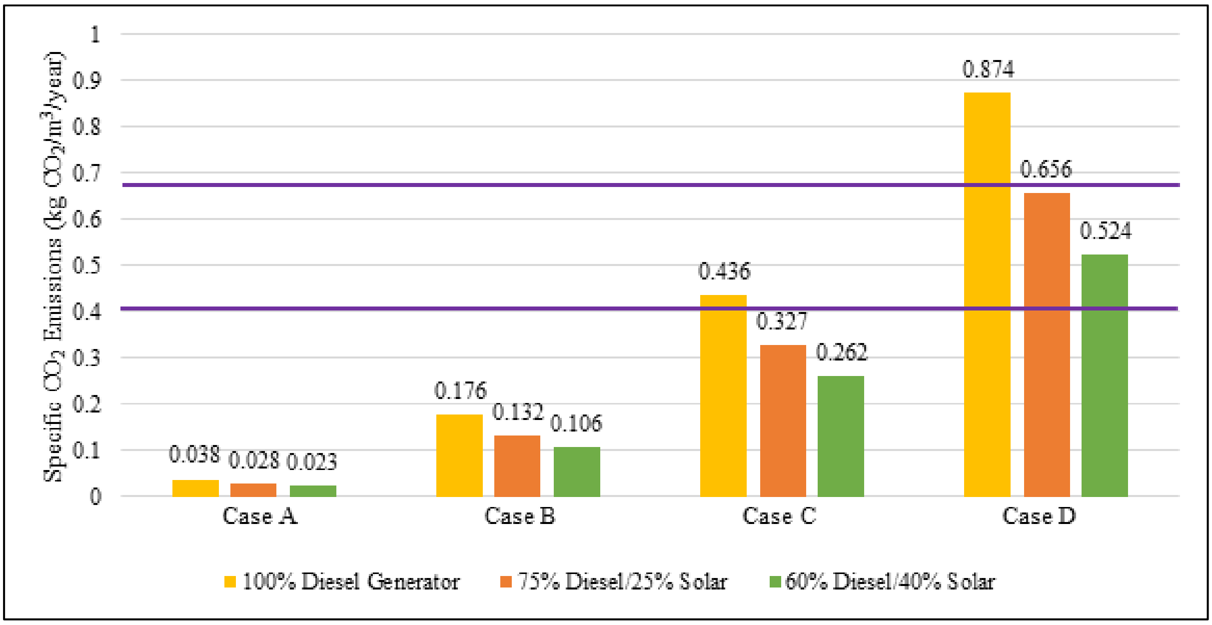


Figure 4.7. Specific CO_2 emissions per case and energy configuration (Bartram et al., 2023)

4.4 Conclusions

Sustainable water desalination should primarily aim towards reducing energy use and CO_2 emissions. Water Application Value Engine (WAVE) and Desalination Economic Evaluation Program (DEEP) software were utilised to analyse and assess reverse osmosis (RO) diesel-solar energy configurations in Oman, from economic and environmental dimensions. It was determined that smaller-scale, modular, intensified RO system designs could be the key towards (green and) sustainable water desalination, particularly with more balanced diesel-solar (i.e. 60-40>75-25) energy configurations. On the other hand, while the specific CO_2 emissions per m^3 of water per year were reasonable in accordance with smaller-scale operations (Figure 4.7), the calculated reductions may have been overstated; diesel generators would not be responsible for all emissions, especially with factors like fuel transportation, and PV maintenance/installation. Furthermore, from an economic perspective, DEEP (or similar software) may potentially overweight labour & management (L&M) costs, which can heavily skew the economic analysis of smaller-scale plant designs. Therefore, it is essential that the desalination software is optimised towards specific scale(s) of operations.

5. Isopropanol (IPA) case study in China

5.1 Overview

A CPP design has been simulated for an IPA synthesis project at the Sinopec Zhenhai Refining & Chemical Co., Ltd., in the Zhenhai District of Ningbo, China. The main raw material was propylene, one of the by-products of a related ethylene company project. An annual plant capacity of 80,000 tons of ultra-pure, electronic-grade IPA was specified, produced (along with 51,000 tons of anhydrous ethanol annually) via the esterification with acetic acid, subsequent hydrogenation, and double-effect distillation. Said IPA has a purity of ~99.99%, while the anhydrous ethanol has a >99.5% purity. The technologies behind the processes were upgraded in accordance with “Made in China 2025 (MIC2025)” green development targets (ISDP, 2018; Wang et al., 2020; Song et al., 2025). Due to its location on one of the company’s reserved development sites, the IPA plant simulation benefits from the following: favourable geography, support from local policies, a plentiful supply of raw material, and well-developed infrastructure (e.g. transportation network). Figure 5.1 illustrates the process flow diagram, with the entire process simulation in Figure 5.2, and the plant layout in Figure 5.3.

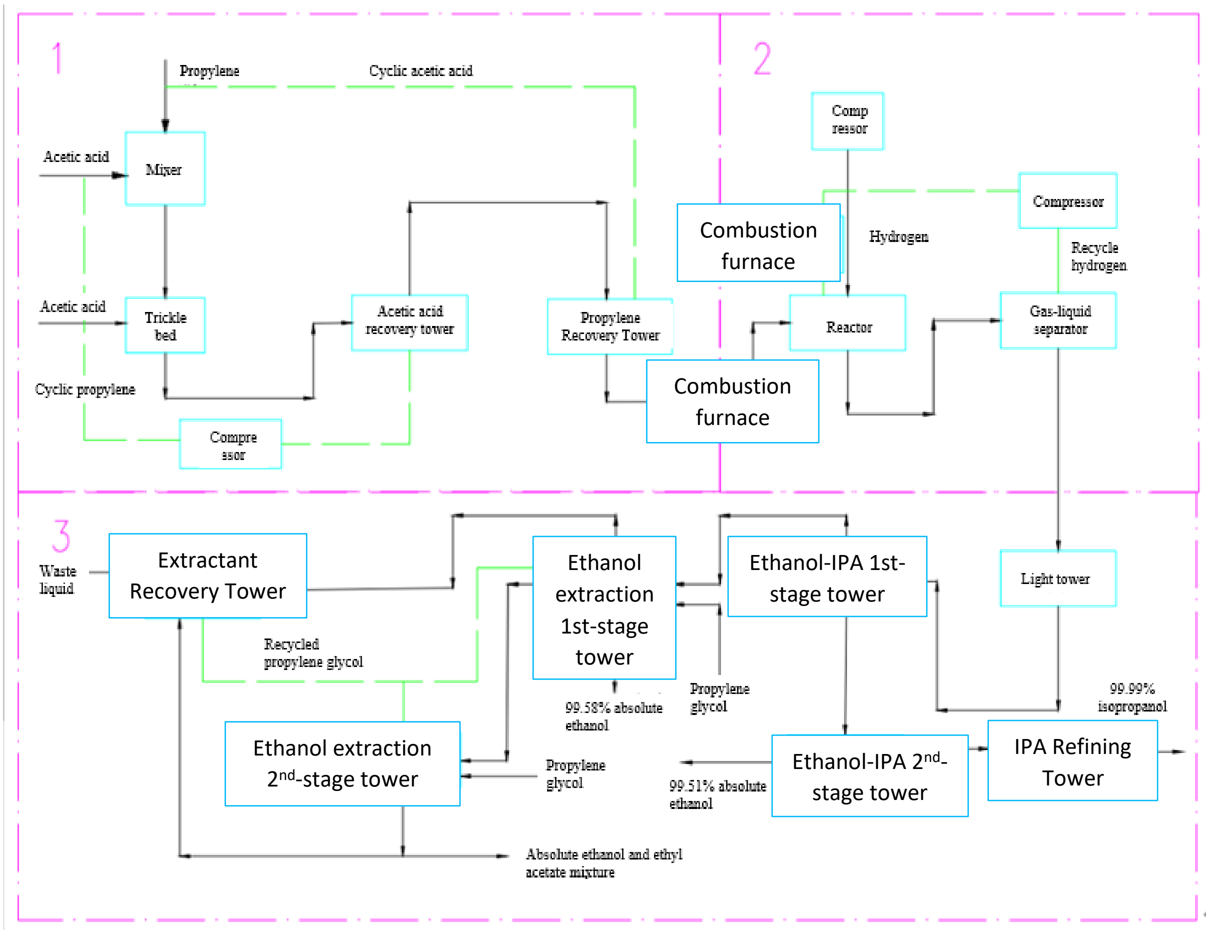


Figure 5.1. Process flow diagram for IPA synthesis via isopropyl acetate. Steps: 1) isopropyl acetate synthesis, 2) isopropanol synthesis, 3) isopropanol & alcohol refinement (Li et al., 2023)

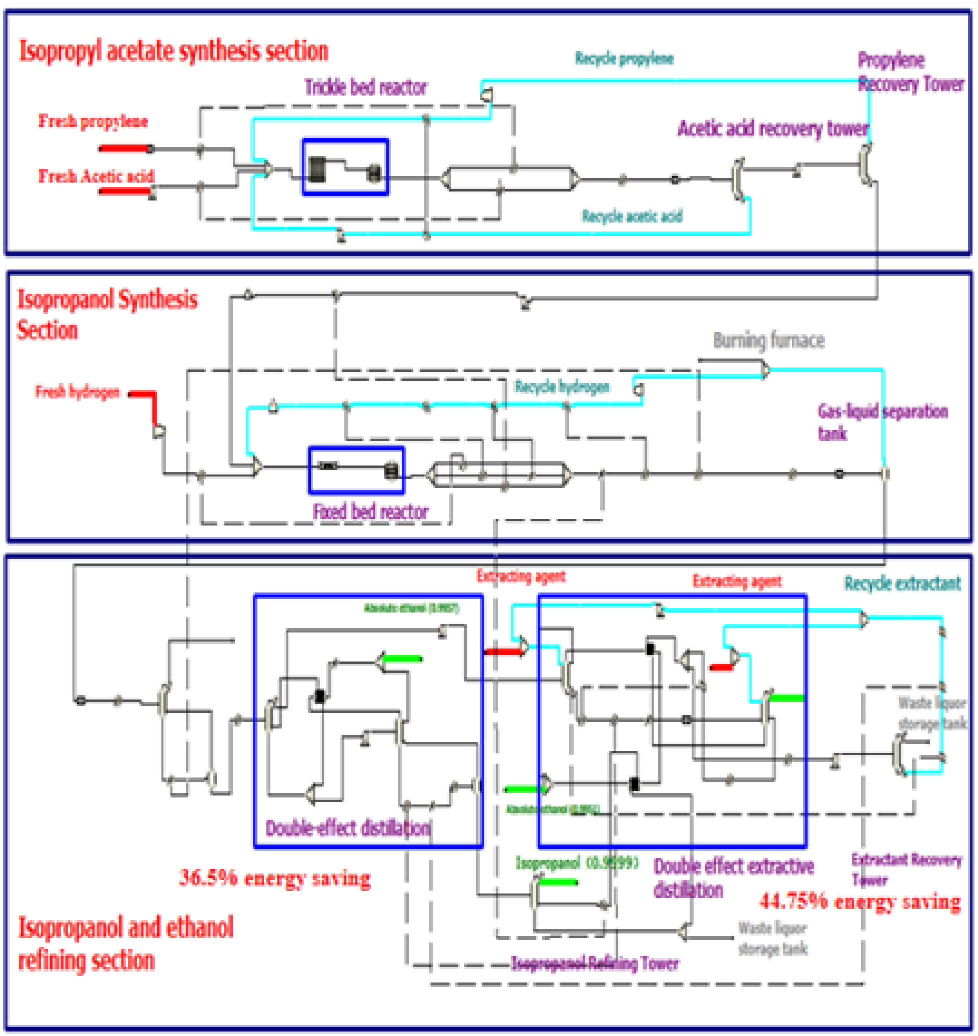


Figure 5.2. Complete top-to-bottom process simulation via Aspen v12. Extraction processes and energy savings have been highlighted per section (Li et al., 2023)

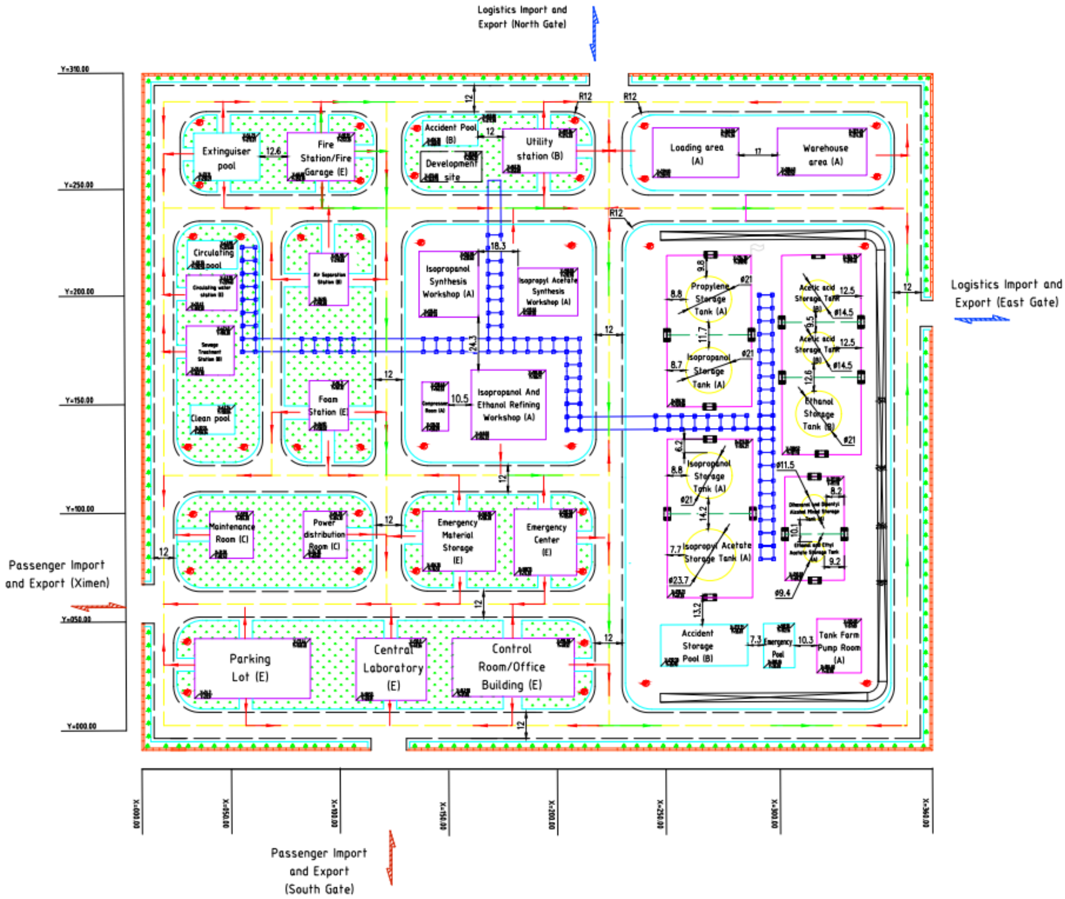


Figure 5.3. Detailed layout of the simulated IPA synthesis plan; passenger imports and exports, safety nodes, and logistics (Li et al., 2023)

Sections 5.2-.4 cover the following key aspects of the proposed IPA process design: economic accounting, environmental assessment, social and political dimensions, and safety evaluation.

5.2 Economic accounting

Costs and prices associated with calculations for non-standard equipment and utility services were derived from publicly available data of the proposed project location (Sinopec Group, 2016). The financial report consisted of a cash flow statement, dynamic indicators (such as the net present value, NPV), and static indicators. Song (2012) outlines the calculation methodology that was utilised, with Chinese Yuan (RMB) as the primary unit of currency, and USD as the reference unit. Moreover, uncertainty analysis was employed, in the forms of break-even and sensitivity analyses (sections 5.2.1 and 5.2.2, respectively). Figure 5.4 outlines the project components for total investment, while Table 5.1 illustrates the key economic and technical indicators of the IPA case study.

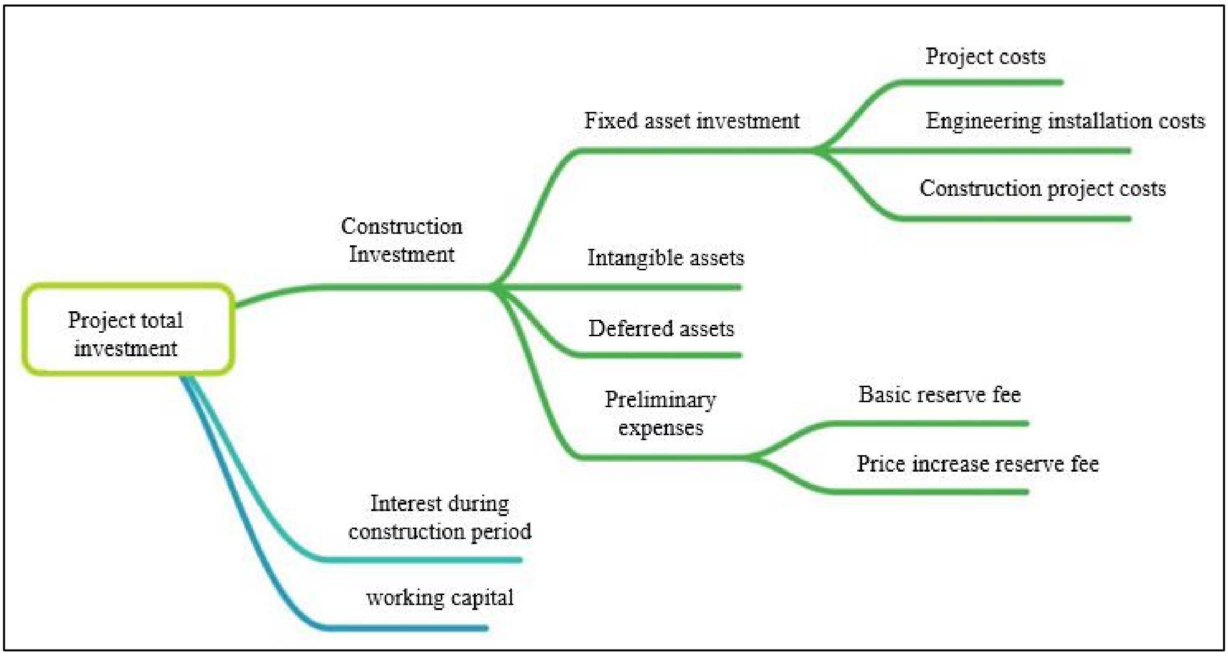


Figure 5.4. Components for total project investment (Li et al., 2023)

Table 5.1. Calculated key economic and technical indicators of the IPA case study (Li et al., 2023)

Number	Project	Unit	Value
I.	**Production scale**	**10,000 tons/year**	**8**
II.	**Product solutions**		
1	Isopropanol	10,000 tons/year	8
2	Ethanol	10,000 tons/year	5.1
3	Isopropyl acetate	10,000 tons/year	0.5
4	A mixture of absolute ethanol and ethyl acetate	10,000 tons/year	1.6
III.	**Years of operation**	**Hour**	**8000**
IV.	**Main raw materials and auxiliary materials consumption**		
1	Propylene	10,000 tons/year	6.52
2	Hydrogen	10,000 tons/year	0.556
3	Acetic acid	10,000	9.32

		tons/year	
6	Glycerol	tons/year	294.9
7	Acidic ion exchange resin	tons/year	0.3
8	Copper zinc catalyst	tons/year	13
V.	**Utility consumption**		
1	-25℃ Frozen brine	10,000 tons/year	80
2	20℃ Cooling water	10,000 tons/year	1200
3	30℃ Air	Nm^3/year	80570
4	Low pressure steam	10,000 tons/year	20
5	Medium pressure steam	10,000 tons/year	5.9
6	High pressure steam	10,000 tons/year	0.996
7	Heat transfer oil	10,000 tons/year	5.59
8	Electricity	10,000 degrees/year	9184
9	Instrument air	Nm3/year	6.5×10^4
VI.	**Waste emissions**		
1	Wastewater	tons/year	3353
2	Exhaust gas	Nm3/h	93.8
3	Waste residue	tons/year	45023.5
VII.	**Factory capacity**	**people**	**100**
VIII.	**Total floor area**	**m2**	**110000**
IX.	Total project investment	10,000 RMB	**26318.12**
1	Construction Investment	10,000 RMB	22603.59
2	Working capital	10,000 RMB	2465.52
3	Interest during construction period	10,000 RMB	1249.01
X.	**Annual sales revenue**	**10,000 RMB**	**152620**
XI.	Costs and fees		

1	Average annual total cost	10,000 RMB	142055.57
2	Average annual operating costs	10,000 RMB	140349.33
XII.	Average annual net profit	10,000 RMB	**11510.19**
XIII.	Financial evaluation indicators		
1	Investment rate of return	%	43.7
2	Investment profit tax rate	%	56
3	Net profit margin on capital	%	32.8
4	Payback period (static)	Year	5.95
5	Payback period (dynamic i=0.13)	Year	8.3
6	Project financial internal rate of return (after tax)	%	23.3
7	Financial net present value (after tax, i=0.13)	10,000 RMB	16153.81
XIV.	Solvency Index		
1	Loan term	Year	6
2	Total loan amount	10,000 RMB	15000
3	Annual repayment amount	10,000 RMB	2945.82

Appendix P provides a full breakdown of cost/price estimations for the reactor equipment, tower equipment, heater equipment, heat exchanger, gas-liquid separator, storage tank, return tank, pump equipment, and compressor (Appendices P-I to P-IX, respectively). Appendix P-X lists the full summary of total process equipment costs. Additionally, Appendix Q-U cover the estimated cost assumptions for the following: total project investment, public works consumptions, employee insurance, depreciation expenses, and taxes.

5.2.1 Break-even analysis

Total revenue is a linear function of unit sales price and the volume of product sales. In contrast, total expenditure is a linear function of unit price and output. This section assumes three things:

1. Constant unit product price throughout the case study's lifespan
2. Quantity of sales = production quantity; all products are sellable
3. Analysed data is representative of a normal production year (Table 5.2)

Table 5.2. First year of production data obtained via accounting (Li et al., 2023)

Project	Value	Unit
Total annual fixed costs(F)	3864.96	10,000 RMB
Comprehensive unit sales price(P)	10315.79	
Variable cost per unit(V)	9091.49	
Unit sales tax(m)	404.27	

Eq.2 is used to calculate the Break-even Point (BEP_Q) of production and sales:

$$BEP_Q = \frac{F}{P - V - m} = \frac{3864.96}{10315.79 - 9091.49 - 404.27} = 4.71$$

(2)

The value for annual project output (4.71 or >47,100 tons) refers to the point at which total income can exceed the total expenditure; i.e., the project becomes profitable. Meanwhile, Eq.3 calculates the maximum allowable reduction in production and sales.

$$\frac{Q - BEP_Q}{Q} x\, 100 = \frac{80{,}000 - 47{,}100}{80{,}000} x\, 100 = 41.13\%$$

(3)

Therefore, the project can be profitable, so long as any reduction(s) in the volume of production and sales does/do not exceed 41.13%. Even the production and sale of relatively low product quantities enables break-even (Figure 5.5) to be attainable, and the production itself to be sustainable. Moreover, the BEP_Q value demonstrates that the IPA case study is overall resilient with great competitive strength, and a strong risk-bearing capacity.

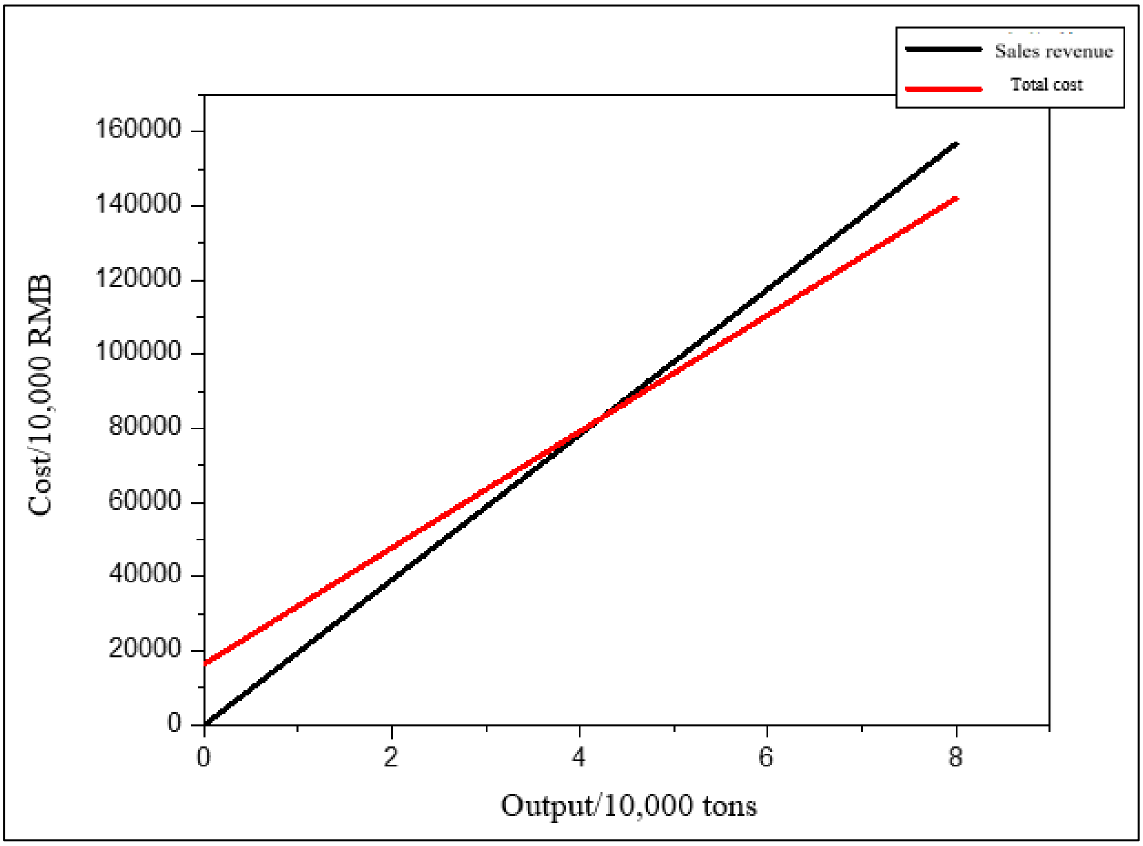


Figure 5.5. Break-even analysis: output vs cost. The intersection of 'sales revenue' and 'total cost' denote the break-even point at 47,100 tons (Li et al., 2023)

5.2.2 Sensitivity analysis

Certain variables were (more) sensitive to change during the calculation period, such as production capacity and/or raw material cost(s). Figure 5.6 illustrates the effect of % alterations in sales revenue and operating costs on NPV. Full details of the sensitivity analyses have been provided in Appendix V-I to V-III, for the following key variables: operating costs, total product output, and product price.

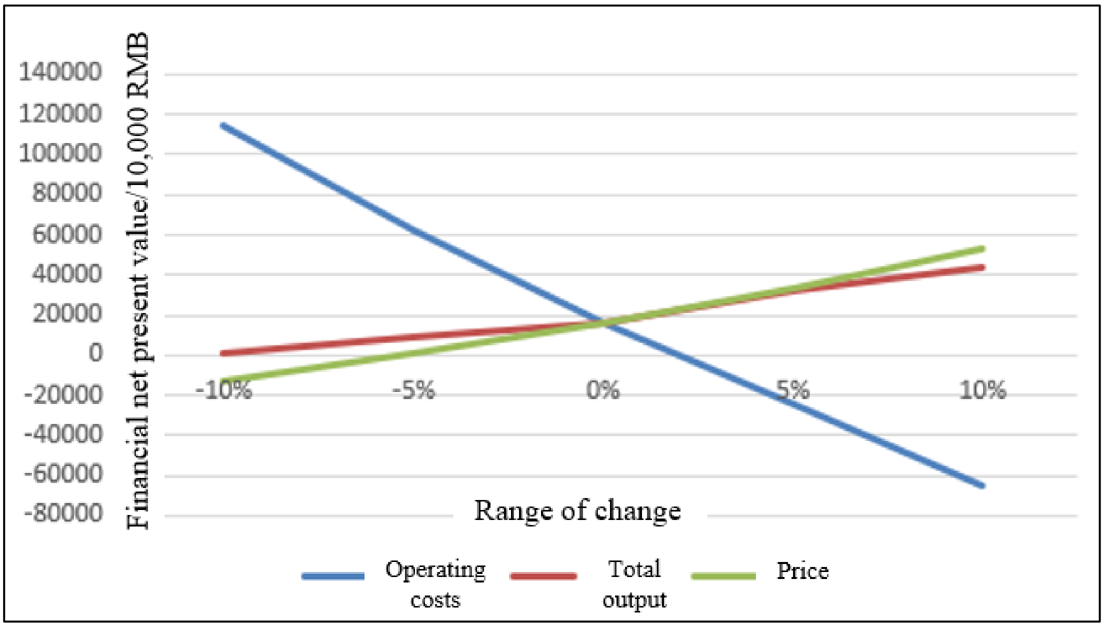


Figure 5.6. Sensitivity analysis of sales revenue and operating costs on NPV and total product output (Li et al., 2023)

It is evidently clear that there is a positive relationship between (product) price and total product output vs NPV. Contrastingly, NPV has a negative relationship with operating costs. Moreover, the impact of operating costs is far more significant than price on NPV, which in turn has a relatively greater impact than total product output. Therefore, operating costs and total product output can be adjusted to effectively address fluctuations in market price, as well as the supply and demand of raw materials and/or products. This also serves to further enhance the case study's overall risk tolerance.

5.3 Environmental assessment

The following environmental assessment involves noise impact evaluation and LCA for the IPA case study, based on standards published by the Ministry of Ecology & Environment of the People's Republic of China (MEEPRC, 2008; Code of China, 2013).

5.3.1 Noise impact evaluation

ELAN20 software was utilised by Li et al. (2023), to computationally estimate the sound power of equipment and acoustic attenuation. Terrain, buildings, ground and air absorption, and sound barriers are key factors considered in the results of acoustic attenuation (Figure 5.7).

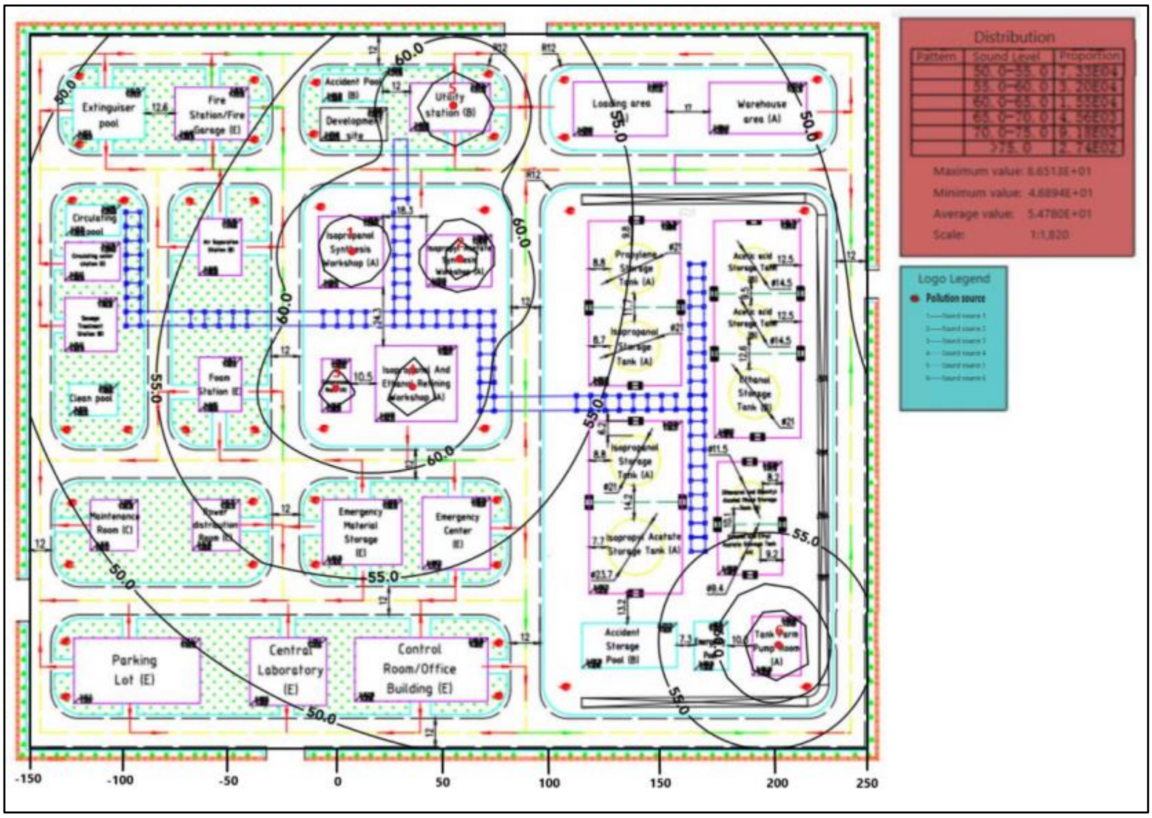


Figure 5.7. Contour distribution map of noise impact evaluation results; noise levels increase with closeness to the central point (Li et al., 2023)

Source co-ordinates are derived via selected reference objects within the plant. Furthermore, sound emission characteristics are derived via operating equipment characteristics. Predictive scheme attributes can then be established; environmental air parameters (e.g., humidity), ground conditions between prediction points and the sound source(s) (e.g., reflections), and definitions for receiving points and obstructions. Figure 5.7 considers the compressors, reaction workshop, and pumps as the main noise sources. The compressor, tank pump, utility stations, and three of the production workshop rooms are regarded as the main sources of noise in the plant layout. Said areas are classified as “high noise zones”, in which noise levels can range between 70-75 dB. Appendices W-I to W-VI elaborate on the following key parameters: site temperature, precipitation, thunder & lightning and frost-free period, humidity and air pressure, wind direction, and wind speed.

A “normal” noise level, akin to a standard office environment, should maintain ~40 decibels (dB). For areas that require relative quiet, such as hospital lounges, <30 dB is the ideal. However, noise levels can vary within a fifteen-metre radius of the site area, from 30 to 50 dB, albeit most of the noise can be sourced to the background environment. Moreover, while high noise zones can reach 70-75 dB, the residential area only experiences 50-55 dB and thus is mostly unaffected. Therefore, in accordance with MEEPRC regulations, the IPA site does not generate significant noise pollution that impacts the surroundings nor the nearby residents. This means that work can be carried out as normal within the site.

5.3.2 Life Cycle Assessment (LCA)

1 kg of IPA served as the representative unit for the LCA (Hossain et al., 2007), which was independent of the MCDM sub-criteria selection process. Due to the plant's location in China, SimaPro 9.4 (with the Ecoinvent 3.8 database) was utilised to conduct the LCA. Evaluation was carried out via the ReCiPe method. Upon completion, the Monte Carlo simulation (running 1000 iterations) was used for uncertainty analysis to determine the statistical parameters of the LCA results (Figure 5.8), such as the confidence intervals, median, and mean. The results suggest that process optimisation is recommended for the IPA distillation process, in which environmental impact and energy consumption were highest.

Figure 5.8. Unlike the bioethanol case study, the LCA results (Li et al., 2023) were not used to derive the key sustainability sub-criteria for the FAHP-TOPSIS framework in Chapter 7

5.4 Social and political dimensions

In addition to employee insurance (Appendix S), and providing over 100 new employment opportunities, safety is a key concern in this case study. Project construction aligns with regional planning standards and national industrial policies, while also promoting rapid industrial chain development. Section 5.4.1 elaborates on site hazards and safety associated with fires and chemicals. Section 5.4.2 links the entire case study to the overall policy implications.

5.4.1 Safety

5.4.1.1 Fire

As per safety regulations (China's State Council, 2012), the IPA case study included fire safety distances (Table 5.3). Figure 5.9 is a visualisation of the plant site layout according to its key functional areas, to evaluate the fire protection layout and its effects on neighbouring businesses.

Table 5.3. Fire safety distances of facilities (Li et al., 2023)

Project facility	Adjacent facilities	Design distance (m)	Requiring distance (m)	Regulations
Fire station	East: the main road in the factory	12	10	3.4.3
	South: The main road in the factory	12	10	3.4.3
	West: Fire Pool	12	5	3.4.3
	North: The main road in the factory	12	10	3.4.3
Syntinicate synthetic workshop	East: the main road in the factory	6	5	3.4.1
	West: isopropanol synthetic workshop	12	12	3.4.1
	South: isopropanol and ethanol refined workshop	12	12	3.4.1
	North: The main road in the factory	15	10	3.4.1
Isopropanol synthetic workshop	East: Syntinate synthetic workshop	15	12	3.4.1
	South: isopropanol and ethanol refined workshop	15	12	3.4.1
	West: Secondary road in the factory	12	12	3.4.3
	North: The main road in the factory	12	10	3.4.1
Isopropanol and ethanol refined workshop	East: the main road in the factory	12	10	3.4.1
	South: The main road in the factory	12	10	3.4.1
	West: The main road in the factory	12	10	3.4.3
	North: Synthetic Synthetic Workshop	15	12	3.4.3
Utilities Station	East: the main road in the factory	10	10	3.4.3
	South: The main road in the factory	10	10	3.4.3
	West: accident pool	12	10	3.4.3
	North: The main road in the factory	10	10	3.4.1

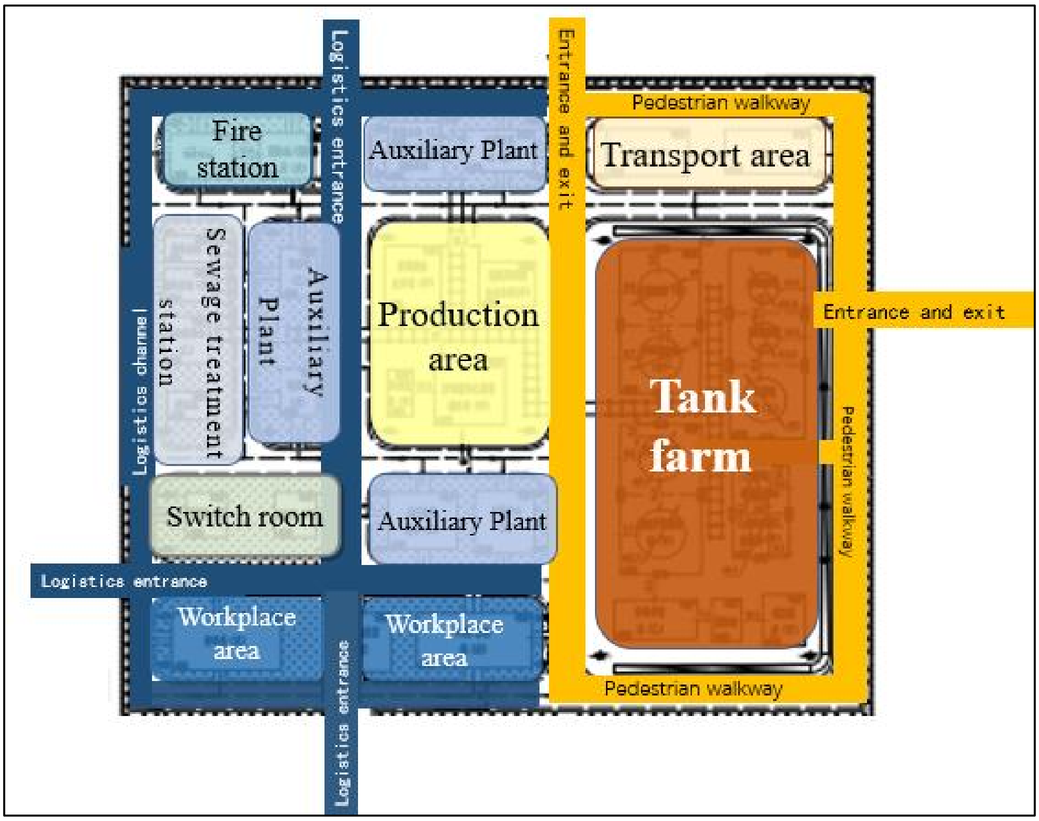


Figure 5.9. Plant site layout according to its key functional areas (Li et al., 2023)

Table 5.4 shows the fire safety distances between the surrounding environment and plant site, in accordance with GB50016 (2018) and GB50016-2014 regulations (China's State Council, 2018). All fire safety distances ensure that site operations can be carried out safely and without harm to the surroundings.

Table 5.4. Safety distances in relation to the surroundings (Li et al., 2023)

Surrounding architecture name		The name of this project facility	Design distance (m)	Requiring distance (m)	Regulations
Position	**Name**				
West	Workspace	Production area (Class A level 1), storage area (Class A level 1)	75	12 25	3.4.1 4.2.1
Southeast part	Residential area	Life Area (Class E level 1)	75	25	4.2.1
Southwest	Zhenhai Steel Refining Factory Auxiliary Production Area	The loading and unloading area, temporary warehouse (Class 1 level)	75	25	3.4.1

Northwest	Zhenhai Refinery	Storage area (Class A level first)	75	25	4.2.1
Northeast	Unsally	Power distribution room, repair station (Class C level 1)	60	25	3.4.1

5.4.1.2 Chemical

Chemical hazard analysis was performed based on the physical properties of each raw material and product (Tables 5.5-.6). Said chemicals could pose significant harm to people and the environment, as well as potentially compromising production and/or storage.

Table 5.5. Chemical hazard analysis (Li et al., 2023)

Item	Dangerous category	Serial number	Fire risk grading	Harmony of vocational contact with poisoning
Propylene	Category 3.1 inflammable gas	21018	Class A	High risk
Hydrogen	Category 2.1 inflammable gas	21001	Class A	High risk
Acetic acid	Category 8.1 flammable liquids	81601	Class A	High risk
Isopropyl	Category 3.2 flammable liquids	32064	Class A	High risk
Ethanol	Category 3.2 flammable liquids	32061	Class A	High risk

Table 5.6. Main risk factor per chemical (Li et al., 2023)

Harmful Substance	Main risk factor	Part
Propylene	Flammable, poisoning	Reactor, distilled tower, storage tank
Hydrogen	Flammable and explosive	Reactor, distillation tower, tank, mechanical transportation
Acetic acid	Flammable, corrosive	Tower, reactors, tanks, mechanical transportation
Isopropyl	Flammable and explosive	Reactor, distilled tower, tank, mechanical transportation
Ethanol	Flammable and explosive	Reactor, distilled tower, tank, mechanical transportation

Due to the flammability of IPA, a major hazard identification assessment was also employed using a Boiling Liquid Expanding Vapour Explosion (BLEVE) software model under GB12268 and GB18218 standards (NSAB, 2012; NSAB, 2018). The BLEVE results for a pool fire simulation. It was determined that storage tanks were adequately spaced, and water in the firefighting pool was sufficient, assuming that operational procedures are normal. Therefore, the site should pose no risk of explosions nor uncontrollable fires, that may endanger the people nor (surrounding) environment. Appendices X-I to X-IV provides a full breakdown of the following: injury range, pool fire simulation model, vapour cloud explosion data, and simulation model for the vapour cloud explosion.

5.4.2 Policy implications

Acetone hydrogenation (AH) was the preferred method to produce IPA, in China. Moreover, the largest IPA synthesiser in China, was found to utilise the AH method at an annual capacity of ~188,000 tons (Table 5.7). Contrastingly, many of the Chinese IPA manufacturers were relatively smaller in scale at 50-60,000 tons/year.

Table 5.7. Major IPA manufacturers in China with >100,000 tons of annual capacity (Li et al., 2023)

Manufacturer	Production scale 10,000 tons/year	Adopt craftsmanship
Shandong Dadi Supu Chemical Industry	10	Acetone hydrogenation
Jinzhou Petrochemical	10	Propylene hydration
Kailing Chemical	18.8	Isopropyl acetate hydrogenation
Lihua Yiweiyuan Chemical Industry	10	Acetone hydrogenation

The simulation case study aimed to diversify the possible methodologies towards IPA synthesis, while also developing a more comprehensive assessment and evaluation framework for future projects in China (or elsewhere). Ideally, this included the consideration of holistically green sustainability and sustainable development.

5.5 Conclusions

An IPA plant at one of the company sites of Sinopec Zhenhai Refining & Chemical Co., Ltd was simulated to uphold the MIC2025 green development targets. The plant simulation has various inherent advantages/benefits, such as its location, infrastructure, and support from local policies. Chapter 5 examines the IPA case study via three key dimensions: economically, environmentally, and socially. Profitability is indeed possible, so long as production is sustainable and any reduction(s) in the volume of production and sales does/do not exceed 41.13%. The IPA plant simulation also exhibits resilience, great competitive strength, and a strong risk-bearing capacity. Environmentally speaking, noise pollution was not regarded as an issue for the plant site, its workers, nor the surroundings. That said, LCA results suggest that process optimisation is recommended for the IPA distillation process, due to its comparatively greater environmental impact.

In terms of the social dimension, hazard analysis was employed under stringent safety regulations, such as GB50016 (2018) and GB18218, for fire and chemical hazards (particularly with regards to IPA). Fire safety distances were deemed sufficient, while a BLEVE model determined that the plant layout itself and facilities meant that explosions and uncontrollable fires were of little risk to people and the environment. However, while this is a comprehensive assessment, future IPA case studies should aim to expand beyond solely safety and policy implications for a truly holistically green and sustainable perspective. Integrated MCDM may be the key towards achieving such a perspective towards CPPs, including IPA synthesis. Sections 7.3-.4 cover the implementation of an integrated FAHP-TOPSIS framework for the prioritisation of holistically green and sustainable IPA pathways.

6. Ammonia production case study

6.1 Overview

Commercial NH_3 production has a rich and extensive history. As the demand for NH_3 has increased, so has the production process (i.e., capacity, efficiency, and so forth) continuously developed. However, as the global population continues to rise and become more urbanised, conventional NH_3 production (with syngas derived from steam-methane reformation; SMR) has become increasingly less viable in the long-term, particularly due to its negative environmental impacts. Therefore, a holistically green and sustainable NH_3 production model must be developed that is also scalable while being (overall) cost-effective. Said green NH_3 production model would rely on Polymer Electrolyte Membrane (PEM) electrolysis for hydrogen generation, which in turn should be powered via renewable energy, such as solar and/or wind power. Aspen Plus v12 has been utilised to create two NH_3 production models: conventional (with SMR) and clean (with PEM electrolysis). And although there is a degree of uncertainty and limitations in total cost estimates, the clean model shows potential towards a scalable, modularised NH_3 production model that is also green and sustainable. But to be truly holistically green and sustainable, all dimensions of green sustainability must be considered equally (or at least, more proportionally).

6.2 Background

NH_3 is arguably the most essential synthetic chemical in the world. It is an intrinsic component of our society, with applications in all aspects of life, from clothing fibres to plastics (Pattabathula & Richardson, 2016; Reese et al., 2016; AIChE, 2020; IEA, 2021). But most importantly, ~90% of all produced NH_3 is used to manufacture fertiliser for crop production (Pattabathula & Richardson, 2016; Reese et al., 2016; AIChE, 2020; IEA, 2021; Lee et al., 2022). Large-scale commercial NH_3 production is carried out via the Haber-Bosch (H-B) process, which was first developed in 1906 by Fritz Haber and Walther Nernst (Allman et al., 2017; Peng et al., 2018; AIChE, 2020; Ozturk & Dincer, 2021). But it was not until 1913, when the first commercial NH_3 plant went on-stream (Pattabathula & Richardson, 2016). And since 1946, NH_3 production capacity has steadily risen to a point where it reached more than 200 Mtonnes/year from 2017 onwards (Nayak-Luke et al., 2018; Lee et al., 2022). Presently, a single train for a "large-scale" NH_3 plant can produce at least 3,300 tonnes/day, while "small-scale" plants can produce at least 50 tonnes/day (Pattabathula & Richardson, 2016; Thyssenkrupp, 2019). Appendix Y provides an overall timeline for NH_3 production.

NH_3 has significant potential as a green, sustainable fuel source and hydrogen energy carrier (Malmali et al., 2016; Allman et al., 2017; Peng et al., 2018), but only if the overall methodology framework is changed to incorporate holistically green sustainability. However, due to the high temperature and pressure requirements, the H-B process is highly energy-intensive and expensive. Said energy is also mostly, if not completely, derived from non-renewable sources, such as fossil-fuels (Pattabathula & Richardson, 2016; Peng et al., 2018; Amhamed et al., 2022). Fossil-fuels release significant amounts of greenhouse gas (GHG) emissions, which contributes to anthropogenic climate change (Reese et al., 2016; Allman et al., 2017). Additionally, the conditions for the H-B process prevents the development of a smaller-scale and more decentralised production framework (Peng et al., 2018). Therefore, NH_3 production must undergo an overall rethinking of process design, including process intensification and shifting paradigms, towards a more green and holistically sustainable perspective.

6.2.1 Current ammonia production

The H-B process is the most commonly used reaction for commercial NH_3 production across the globe (Pattabathula & Richardson, 2016; Peng et al., 2018; Amhamed et al., 2022). The process involves passing a mixture of nitrogen and hydrogen gases through a solid iron-based catalyst at 650-750 K and 50-200 bar, depending on the plant configuration (Vojvodic et al., 2014; Chen et al., 2019; Amhamed et al., 2022; Darmawan et al., 2022). Any unreacted gases that contain nitrogen and/or hydrogen are recycled, to be converted into more NH_3 (Chen et al., 2019; Darmawan et al., 2022). It is a reversable reaction, as displayed in Eq.4:

$$\mathbf{N_2 + 3H_2 \leftrightarrow 2NH_3} \tag{4}$$

In the 21st century, the market for NH_3 plant technology is dominated by the following three suppliers: ThyssenKrupp Industrial Solutions (TKIS), Kellogg Brown & Root (KBR), and Haldor Topsøe (Pattabathula & Richardson, 2016). Moreover, modern NH_3 plants have become increasingly more efficient, in terms of energy, production, and safety. In comparison to coke-based plants and the first plants based on natural gas, which required 60 gigajoules per metric ton (GJ/mton of energy) and 40-50 GJ/mton, respectively, 28 GJ/mton is consumed by the most efficient modern NH_3 plants (Pattabathula & Richardson, 2016). Heat and hydrogen recovery is also integrated into modern plants, further lowering energy requirements and capital costs, while also improving production (Pattabathula & Richardson, 2016; Allman et al., 2017; Peng et al., 2018). Furthermore, in addition to more efficient technologies, process design changes have increased NH_3 concentrations, from the initial 6% concentration achieved in 1906, to 19-21% concentrations in present day (Pattabathula & Richardson, 2016). Changes include the implementation horizontal/radial catalyst beds, cheaper and less resource-intensive NH_3 production, more efficient turbines and/or compressors, and so forth (Pattabathula & Richardson, 2016; Stasiulaitiene et al., 2016; Peng et al., 2018).

However, the most conventional H-B process with hydrogen production via SMR, still requires large capital investment(s) and high energy requirements, from which the energy and hydrogen feedstock is mostly derived (~95%) from the burning of non-renewable fossil-fuels (Pattabathula & Richardson, 2016; Nayak-Luke et al., 2018; Peng et al., 2018; Ozturk & Dincer, 2021; Amhamed et al., 2022). NH_3 production via the H-B process with SMR constitutes 1-2% of global energy consumption and releases significant amounts of greenhouse gas (GHG) emissions; 235 Mtonnes/year of CO_2 emissions, with 80% of the emissions via the SMR process (Patil et al., 2016; Reese et al., 2016; Allman et al., 2017; Nayak-Luke et al., 2018; Lee et al., 2022). As the global population (and thus demand for NH_3) increases, the eventual reduction of GHG emissions via improvements in energy efficiency may not be sufficient (IEA, 2021). By 2050, global NH_3 production is predicted to increase to 270 Mtonnes/year (Nayak-Luke et al., 2018).

Therefore, it is imperative that NH_3 production becomes green, sustainable, and overall (more) cost-effective. Previous studies have shown that there is immense potential to achieve said goals, starting with the decarbonisation of the hydrogen production process, and increasing interest from major investors (Nayak-Luke et al., 2018; IEA, 2021; Ozturk & Dincer, 2021; Lee et al., 2022). A transition towards renewable energy sources—such as wind power for electricity generation—for NH_3 production is essential, in addition to plant scalability and performance from an economic perspective (Malmali et al., 2016; Reese et al., 2016; Allman et al., 2017). Additionally, NH_3 production should expand its social scope, which is primarily limited to safety, if discussed at all (Pattabathula & Richardson, 2016; Allman et al., 2017). A holistically green and sustainable NH_3 production framework should also consider other social aspects in chemical process design, such as the effects on energy security, and social acceptability.

6.2.2 Project confinements

Project confinements were subject to frequent changes, particularly as the project had progressed. Even so, several key confinements were identified. The NH_3 plant was designed to involve a "numbering-up" approach for its WPD with smaller and stackable unit-scale modules in parallel, in order to produce the required quantity of throughput. Moreover, innovative designs throughout the process design were desired, to minimise the amount of background intellectual property (IP) that would have required licensing. And, wherever possible in the WPD, process intensification concepts were implemented to minimise techno-economic and environmental costs; e.g. total equipment costs and GHG emissions. The project also assumed that ~50 mton/day was the most appropriate capacity for continuous, year-round operation. Additionally, it was assumed that seasonal variations in fertiliser demand can/would be levelled out via various off-take agreements; for example, via sales to a neighbouring facility that converts NH_3 to other, storage-friendly forms of fixed nitrogen outside of the growing season.

Any decisions and recommendation for the WPD also had to be approached from a holistic perspective, in terms of the following dimensions: social, safety, economic, financial, technical, and environmental. This involved minimising the process design's overall carbon footprint, while under the assumption that the proposed system would have a 20-year useful plant life. A 20-year plant life assumption was derived for the purposes of economic analysis, in conjunction with the assumption that the internal rate of return (IRR) would have been calculated from the payback analysis to derive an acceptable NPV.

6.3 NH_3 production

A biomass case study acted as the initial placeholder case study, to validate the overall methodology framework. As part of the project's overall methodology, two integrated MCDM frameworks (FAHP-TOPSIS and FAHP-VIKOR with PROMETHEE-II), under a WPD philosophy, were proposed with modularised (green) NH_3 production as a case study. Both frameworks were designed to be applicable to any CPP design with relative flexibility. According to AIChE (2020), NH_3 production accounts for 1-3% of global energy consumption, ~3% of global GHG emissions, and 5% of natural gas consumption; this is only expected to increase with a growing (and more urbanised) global population (Patil et al., 2016; Allman et al., 2017). Modularised processing enabled the methodology frameworks to be more flexible and distributable (Dahlgren et al., 2013; Grieco, 2019), from holistically green and sustainable perspectives.

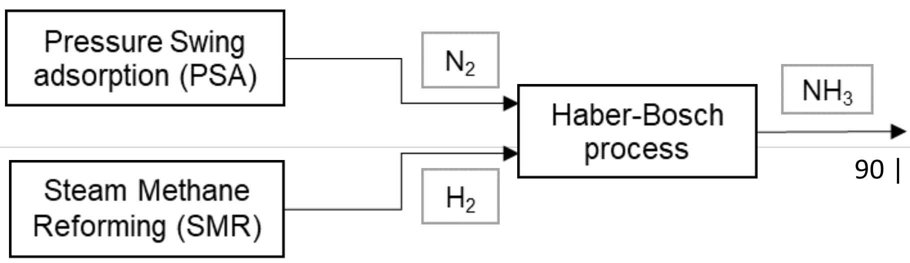
Two NH_3 production simulation models were analysed, with emphasis on production capacities, potential scalability, and estimated costs; 1) NH_3 production via syngas as feedstock, from SMR-derived hydrogen and nitrogen via the air; 2) hydrogen via electrolysis and nitrogen from an air separation unit (ASU). Moreover, the project had incorporated clean and renewable electricity to fulfil the high energy demands associated with NH_3 production.

6.4 Materials & Methods

The NH_3 production process for each case study was modelled in the latest version of Aspen Plus (v12.8, at the time of writing). All the case studies followed the same steps to set up the Aspen Plus model:

1) Create the component list
2) Select the property method
3) Define the reaction(s) and/or reaction set(s)
4) Create the flowsheet
5) Input the parameters for each component
6) Run the model

Figure 6.1 shows the block flow diagrams for the case studies: the H-B process using SMR vs Polymer Electrolyte Membrane (PEM) electrolysis for hydrogen generation (top and bottom, respectively).



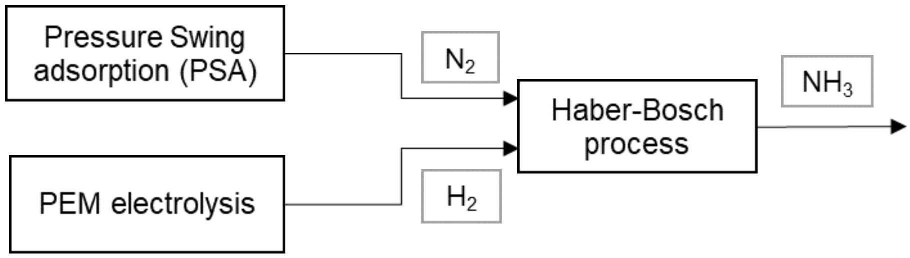


Figure 6.1. Block flow diagrams for the H-B process with conventional SMR (top) vs "clean" PEM electrolysis (bottom) coupled with their respective ASU technologies

6.4.1 Scope boundaries

For the purposes of ease and practicality, the conventional method of NH_3 production had focused solely on the modelling of the NH_3 production module (section 6.4.2.1). Therefore, only one reaction had to be defined in Aspen Plus v12, with a standard 3:1 stoichiometric ratio for hydrogen and nitrogen, respectively (Eq.4).

In contrast, the green "clean" NH_3 production model is fully illustrated and explained in sections 6.4.2.2-.5, in three modules: hydrogen generation, nitrogen generation, and NH_3 synthesis. More novel approaches to NH_3 production, such as non-thermal plasma-assisted technologies, were not explored in this case study. This was mainly due to maturity of the H-B process, as well as its comparatively greater potential for near-future scalability.

6.4.2 Process simulation models

6.4.2.1 Conventional ammonia production via syngas

The following components were selected to constitute the component list: nitrogen (N_2), hydrogen (H_2), ammonia (NH_3), carbon dioxide (CO_2), methane (CH_4), carbon monoxide (CO), and water (H_2O). Redlich-Kwong-Soave Modification (RKS-BM) equation of state was selected as the property method, as it is one of the most commonly used for ammonia production. Moreover, the standard 3:1 ratio between H_2 and N_2 was decided for the reaction, R-1.

Figure 6.2 illustrates the model flowsheet for a conventional NH_3 production module, modified from the low-pressure and low-temperature system developed by Al-Malah et al. (2018), while using some of the model data from Frattini et al. (2016). Prior to pressurisation in the multi-stage compressor (MSCMP), the SYNGAS was processed through a syngas clean-up unit. The feedstream entered the process simulation model at 280°C and 26.52 bar, with a total flow rate of 7000 kmol/hr. Two feedstream datasets were applied to SYNGAS, to test and validate the model (Table 6.1).

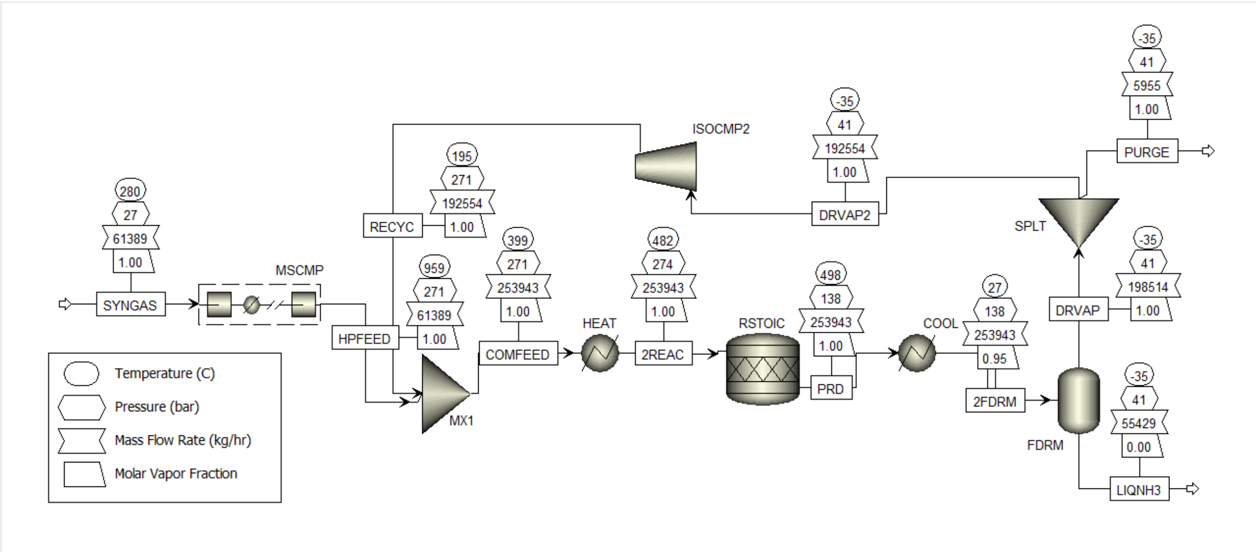


Figure 6.2. Conventional NH_3 production via syngas that was processed through a syngas clean-up unit (Al-Malah et al., 2018)

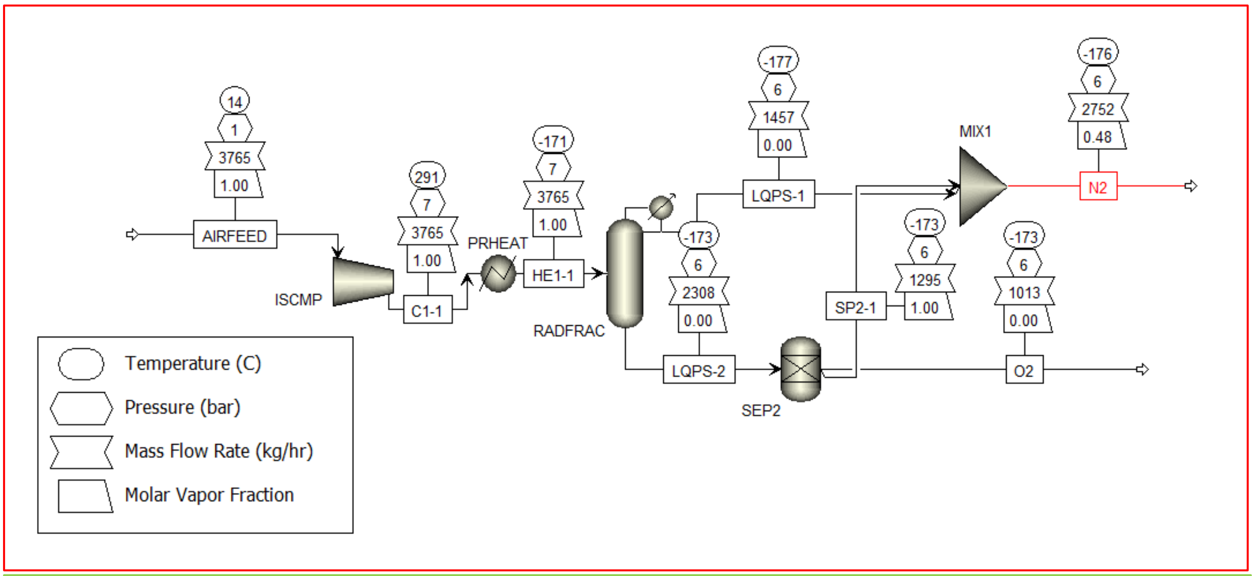
Table 6.1. Syngas feedstream datasets. Dataset 2 substituted the guide's use of argon with CO_2 (Frattini et al., 2016)

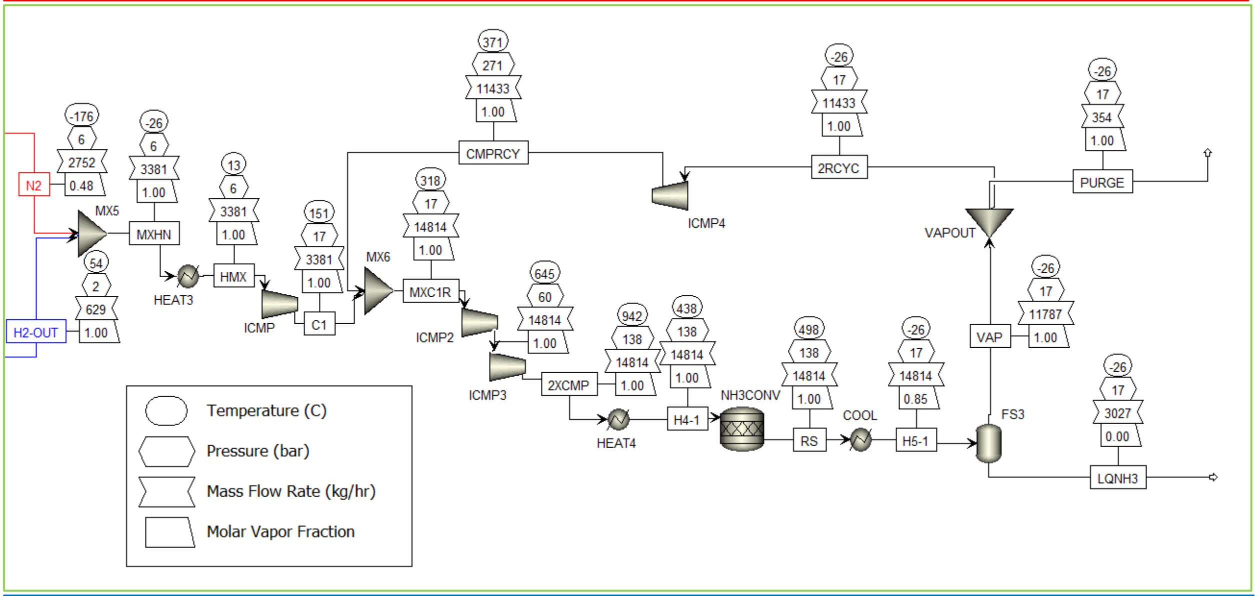
Component	Dataset 1 (Frattini et al., 2016) (mol%)	Dataset 2 (Aspen Plus v8.0 NH_3 guide) (mol%)
N_2	7.80	24.74
H_2	21.00	73.71
CH_4	3.50	1.03
CO_2	8.20	0.28
CO	11.50	0.24
H_2O	48.00	0.00

MCOMP had elevated the pressure to 271 bar, before the now highly pressurised feedstream (HPFEED) was sent to the mixer (MX1). The combined feed was then heated in the heater, HEAT, to the reaction temperature of 498°C, while pressure was altered to 138 bar. A stoichiometric reactor (RSTOIC) was chosen for the reactor, with a fractional conversion of 0.3 of the H_2 component in equation 1. The next step involved cooling the stream in COOL, the cooler, where temperature was lowered to -35°C at 40.53 bar, in preparation for the flashing process in FDRM. FDRM is a flash drum, which was modelled with a 'flash2' type separator in Aspen Plus. ~99% of the final liquid product was composed of pure NH_3. And, of the ~1% of drum-off vapour, 3% was released as PURGE via a splitter (SPLT). The rest (i.e., 97% of the drum-off vapour) was transferred to the second isentropic compressor (ISOCMP2) for recycling. ISOCMP2 had applied a pressure of 271.4 bar to the recycled stream, before it was then returned to MX1 and mixed with the HPFEED.

6.4.2.2 Clean NH_3 production via electrolysis

Peng-Robinson (PENG-ROB) equation of state was selected as the property method/package in Aspen Plus, because of its high reliability and applicability to various system types. This includes (relatively) non-ideal systems, in contrast to the Soave-Redlich-Kwong equation (AspenTech, 2013). The standard 3:1 ratio between H_2 and N_2 was decided for the reaction, R-1, to synthesise liquid NH_3. The flowsheet model for clean NH_3 production (Figure 6.3) via electrolysis can be divided into three 'modules', all developed by Arrarte (2022): gaseous hydrogen generation via the desalinisation of seawater coupled with PEM electrolysis (Figure 6.4), gaseous nitrogen via ASU that utilises a cryogenic distillation process (Figure 6.5), and NH_3 synthesis (Figure 6.6).


14
1
3765
1.00
AIRFEED
ISCMP
291
7
3765
1.00
C1-1
PRHEAT
-171
7
3765
1.00
HE1-1
RADFRAC
-177
6
1457
0.00
LQPS-1
-173
6
2308
0.00
LQPS-2
SEP2
-173
6
1295
1.00
SP2-1
MIX1
-176
6
2752
0.48
N2
-173
6
1013
0.00
O2
Temperature (C)
Pressure (bar)
Mass Flow Rate (kg/hr)
Molar Vapor Fraction


-176
6
2752
0.48
N2
MX5
54
2
629
1.00
H2-OUT
-26
6
3381
1.00
MXHN
HEAT3
13
6
3381
1.00
HMX
ICMP
151
17
3381
1.00
C1
MX6
318
17
14814
1.00
MXC1R
ICMP2
645
60
14814
1.00
ICMP3
942
138
14814
1.00
2XCMP
HEAT4
438
138
14814
1.00
H4-1
NH3CONV
498
138
14814
1.00
RS
COOL
-26
17
14814
0.85
H5-1
FS3
-26
17
3027
0.00
LQNH3
-26
17
11787
1.00
VAP
VAPOUT
-26
17
354
1.00
PURGE
-26
17
11433
1.00
2RCYC
ICMP4
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271
11433
1.00
CMPRCY
Temperature (C)
Pressure (bar)
Mass Flow Rate (kg/hr)
Molar Vapor Fraction

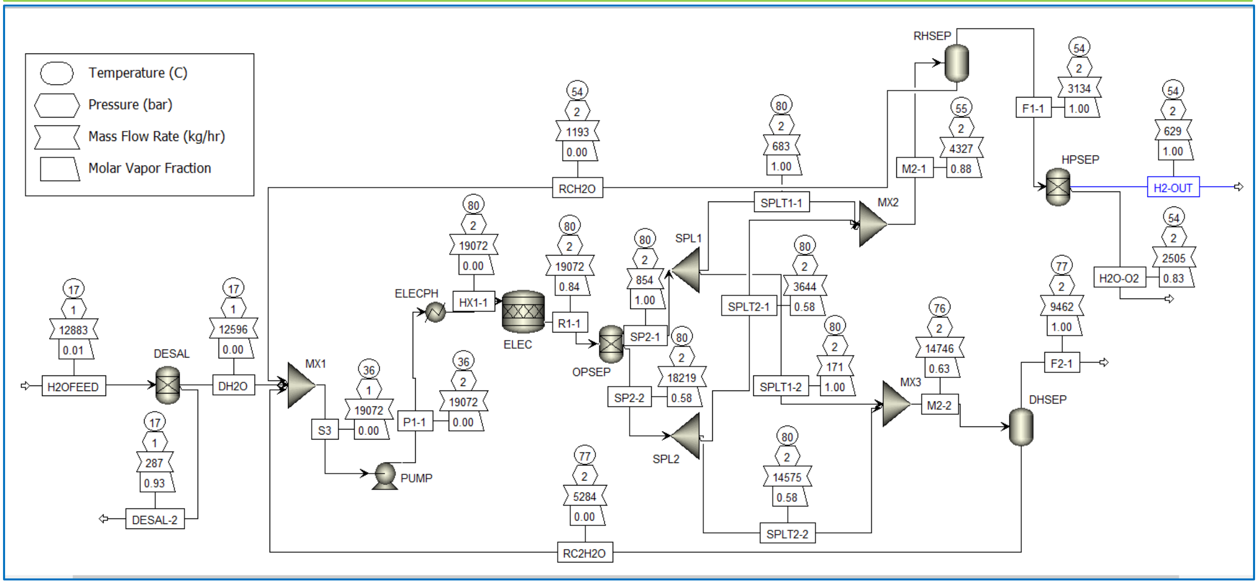
Temperature (C)
Pressure (bar)
Mass Flow Rate (kg/hr)
Molar Vapor Fraction
17
1
12883
0.01
H2OFEED
DESAL
17
1
287
0.93
DESAL-2
17
1
12596
0.00
DH2O
MX1
36
1
19072
0.00
S3
PUMP
36
2
19072
0.00
P1-1
ELECPH
80
2
19072
0.00
HX1-1
ELEC
80
2
19072
0.84
R1-1
OPSEP
80
2
854
1.00
SP2-1
SPL1
80
2
18219
0.58
SP2-2
SPL2
80
2
3644
0.58
SPLT2-1
80
2
171
1.00
SPLT1-2
80
2
683
1.00
SPLT1-1
80
2
14575
0.58
SPLT2-2
MX2
55
2
4327
0.88
M2-1
RHSEP
54
2
3134
1.00
F1-1
54
2
1193
0.00
RCH2O
HPSEP
54
2
629
1.00
H2-OUT
54
2
2505
0.83
H2O-O2
MX3
76
2
14746
0.63
M2-2
DHSEP
77
2
9462
1.00
F2-1
77
2
5284
0.00
RC2H2O

Figure 6.3. Clean NH_3 production flowsheet model. Three modules: hydrogen generation (blue), nitrogen generation (red), NH_3 production (green). 'H2-OUT' (blue) and 'N2' (red) streams were the input streams for the NH_3 production module

6.4.2.3 Hydrogen generation module

The following components were selected to constitute the component list: N_2, H_2, H_2O, oxygen (O_2), potassium (K), magnesium (Mg), calcium (Ca), sodium ions (Na^+), chloride ions (Cl^-), and sulphate ions (SO_4^{2-}). Seawater (H2OFEED) enters the desalinisation unit (DESAL) at 16.5ºC and 1 bar, with a total mass flow rate of 12910 kg/hr. Figure 6.4 shows the model flowsheet for the H_2 generation process via PEM electrolysis from desalinised H_2O. The mole fractions for each component that had constituted H2OFEED are provided in Table 6.2.

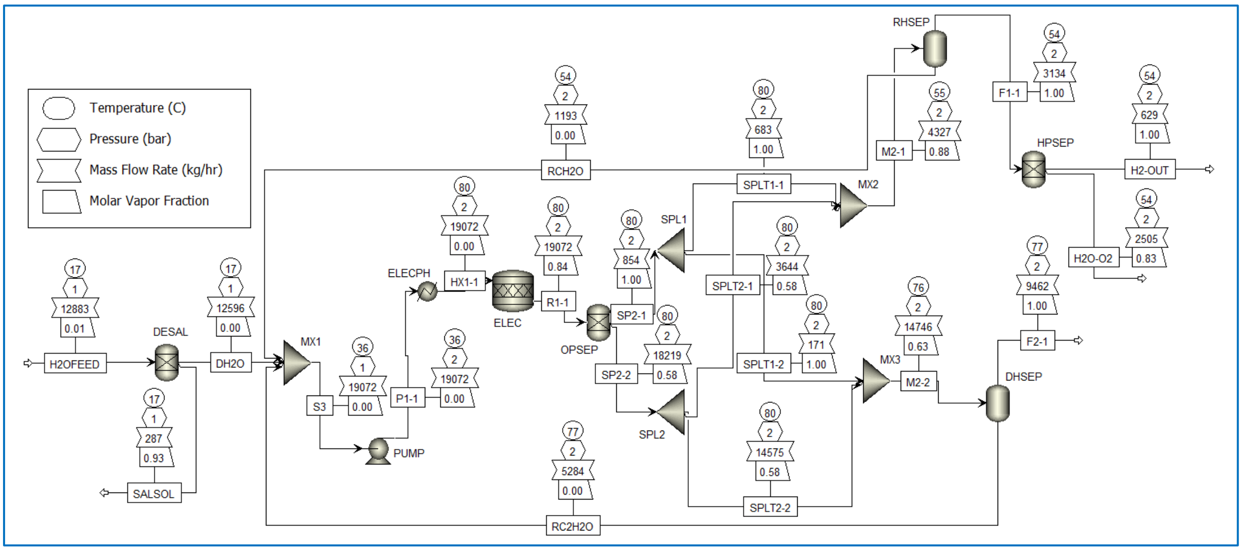

Figure 6.4. H_2 generation via the desalinisation of seawater coupled with PEM electrolysis

Table 6.2. H2OFEED feedstream components and their respective mole fractions (Arrarte, 2022)

Component	Mole fractions (mol%)
N_2	0.000
H_2	0.000
H_2O	98.908
O_2	0.000
K	0.0155
Mg	0.031
Ca	0.0155
Na^+	0.387
Cl^-	0.465
SO_4^{2-}	0.178

DESAL was simulated with a 'flash2' type separator. In order for the subsequent stacks in the model to properly function as intended, the DH2O stream had to have a split fraction value of 1 for H_2O. Resultantly, only desalinised H_2O was allowed to reach the mixer (MX1). Once it had been mixed with the recycled H_2O streams (RCH2O and RC2H2O), the stream was sent to the pump (PUMP), which had had a discharge pressure of 1.5 bar. ELECPH served as the electrolyser pre-heater, which heated up the H_2O to 80ºC at 1.5 bar. This prepared the stream to be transferred to the electrolyser (ELEC), which had been modelled using a stoichiometric reactor (RSTOIC). Said reactor had the following equation (Eq.5):

$$2H_2O \rightarrow 2H_2 + O_2 \tag{5}$$

ELEC split HO into H_2 and O_2, with a fractional conversion of 0.5 of the H_2O. Any remaining H_2O that had left the cell stack was then split from the gaseous O_2 via the oxygen phase separator, OPSEP. This was represented by 'sep' type separator. Each splitter (SPL1 and SPL2) had a split fraction value of 0.8 for streams SPLIT1-1 and SPLIT2-2, respectively. Said streams were then combined in mixers MX2 and MX3 with SPLIT2-1 and SPLIT1-2, respectively. The resultant streams (M2-1 and M2-2, respectively) were transferred to their respective flash units, RHSEP and DHSEP. Both were represented by 'flash2' type separators. RHSEP separated H_2O from H_2-rich steam (F1-1) at 54ºC and 1.5 bar, while DHSEP separated H_2O from H_2-deficient/non-rich steam (F2-1) at 77ºC and 1.5 bar.

The final step involved a hydrogen phase separator (HPSEP), in which H_2O was separated from gaseous H_2 to generate a near-pure H_2 feedstream (H2-OUT) for the NH_3 synthesis module. SP3 had the split fraction of 0.8 for H_2, as well as 0.02 for O_2 and H_2O.

6.4.2.4 Nitrogen generation module

The following components were selected to constitute the component list: N_2, H_2O, O_2, and argon (Ar). Air (AIRFEED) had entered the isentropic compressor (ISCMP) at 13.5ºC and 1 bar, with a total mass flow rate of 3765 kg/hr. Figure 6.5 is the model flowsheet for the N_2 generation via an ASU that had utilised a cryogenic distillation process. The mole fractions for each component that had constituted AIRFEED are listed below in Table 6.3.

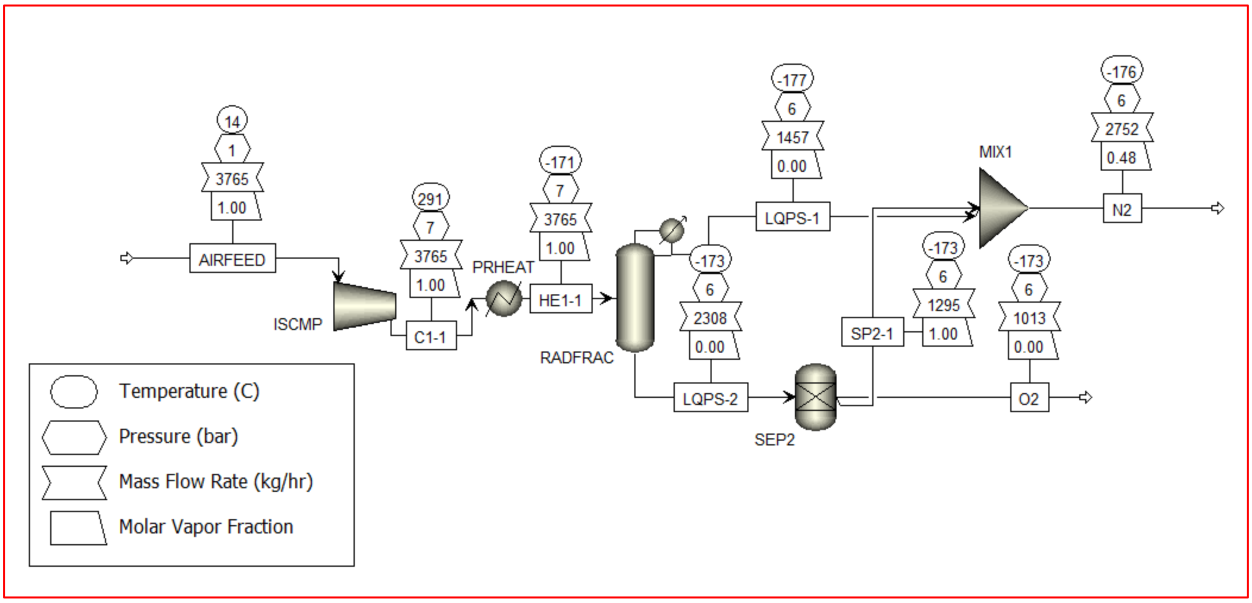

Figure 6.5. N_2 generation via an air separation unit (ASU)

Table 6.3. AIRFEED feedstream components and their respective mole fractions (Arrarte, 2022)

Component	Mole fractions (mol%)
N_2	78.118
Ar	0.932
H_2O	0.000
O_2	20.950

The compressed air feed was sent to a pre-heater (PRHEAT) that had a pressure of 6.5 bar, and a vapour fraction of 1. RADFRAC and SEP2 simulated the core of the air separation equipment via two-stage, high-and-low pressure rectification. RADFRAC was a 60-on-stage 'RadFrac' column model without a reboiler, in which HE1-1 underwent equilibrium distillation at a 0.4 distillate-to-feed (D:F) ratio. Additionally, condenser pressure (i.e. stage 1) was set to 6 bar. Liquid phase streams, LQPS-1 and LQPS-2, were produced as the outputs. SEP2 split fractions were set to 0.9 for N_2, and 0.05 for Ar and O_2. LQPS-1 and SP2-1 were then mixed in MIX1 to generate the required N_2 feedstream for the NH_3 synthesis module.

6.4.2.5 Ammonia synthesis

The following components were selected to constitute the component list: N_2, H_2, NH_3, Ar, O_2, and H_2O. Figure 6.6 shows the model flowsheet for the clean NH_3 synthesis module, using the H_2 and N_2 outputs from Figures 6.4 and 6.5, respectively, as the feedstreams (H2-OUT and N2). The synthesis module developed by Arrarte (2022) was modified to include a more conventional closed synthesis loop. This was due to the limited capabilities of Aspen Plus, as it is unable to include a shell-and-tube heat exchanger without the additional use of 'Aspen Exchanger Design & Rating'.

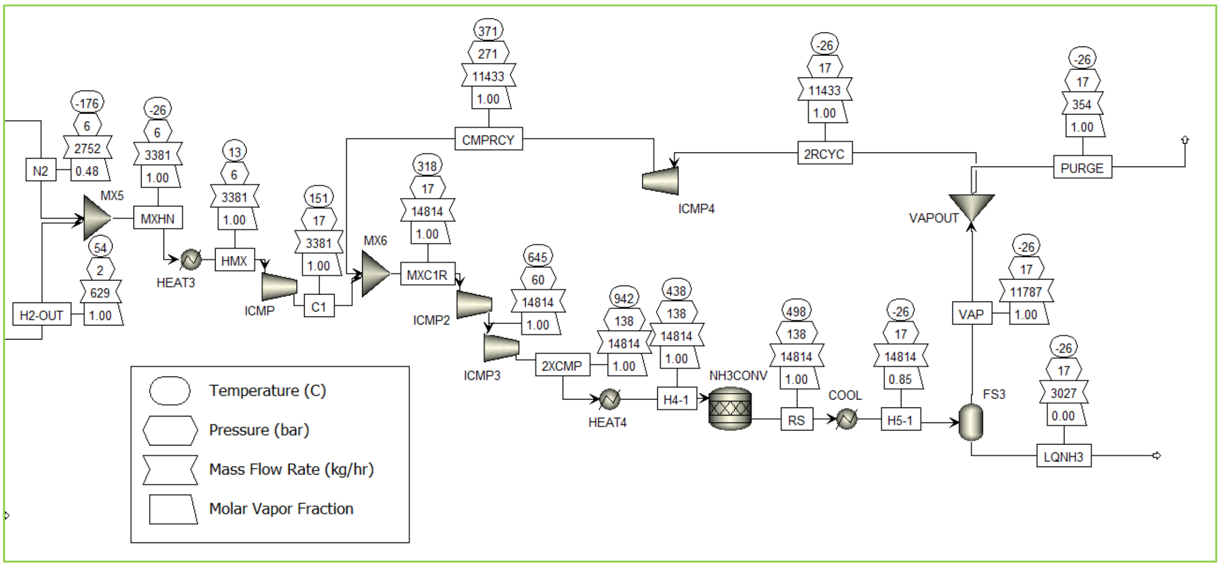

Figure 6.6. NH_3 synthesis module flowsheet

The N_2 and H_2 feedstreams were mixed in MX5, to be subsequently heated up in HEAT3 (-0.01 bar and vapour fraction=1), to avoid any liquid in the isentropic compressor (ICMP), with a discharge pressure of 17 bar. MX6 combined the recycle stream with the output of ICMP (C1) to produce MXC1R. MXC1R was then run through adiabatic compressors, ICMP2 and ICMP3, which were simulated by standard isentropic compressors at 60 and 138 bar, respectively. HEAT4 had prepared the inlet stream by heating it up to 438°C (and -0.1 bar), before it was transferred to the NH_3 converter (NH3CONV). A NH_3 converter was simulated using a stoichiometric reactor (RSTOIC) with equation 1 for the reaction at 438°C and 138 bar. The resultant stream (RS) was cooled in COOL at -26°C and 17 bar, before it was sent to the flash separator (FS3) to obtain the final product, liquid NH_3. VAPOUT split the vapour outlet (VAP), that has been separated to be recycled, and created a PURGE stream. Said PURGE split fraction was 0.03. VAP represented the recycle stream before its compression in ICMP4, an isentropic compressor, at 271 bar. The compressed recycle stream (CMPRCY) was then transferred to the MX6 to be mixed with the feedstreams.

6.4.3 Cost calculations

Even though Aspen Plus v12.0 has a built-in stream price calculator, a series of manual calculations had to be carried out to ensure the correct input values. Furthermore, up-to-date unit prices per kg for components had to be applied into the stream calculations (Table 6.4).

Table 6.4. Unit prices per kg (in USD) for each relevant stream component

Component	USD Unit price per kg (date)
N_2	2.48 (2023)
H_2	1.60 (grey, 2022); (green)
NH_3	1.115 (2023)
CH_4	0.704 (2023)

Equipment cost estimates were more difficult to ascertain, as Aspen Plus had required additional software packages, such as 'Aspen Process Economic Analyzer' or similar non-free alternatives. Such economic-analysis software platforms could have provided more accurate, precise, and in-depth utility cost calculations. The information and calculations are detailed in the sub-sections 6.4.3.1-.2.

6.4.3.1 Conventional

6.4.3.1.1 Stream data

Stream costs were calculated in USD$/kg and subsequently converted into USD$/tonne. Due to the lack of reliable unit cost information for CO and CO_2, and the relatively negligent content in SYNGAS, they were ignored in the cost calculations. According to the International Energy Agency (IEA), the average global levelised cost of 'grey' H_2 generation (i.e. via SMR) in 2022 is $1.6/kg or $1600/tonne (IEA, 2022). In comparison, the unit price of N_2 was $2/litre in 2023 (University of Arkansas, 2023), which was converted into $2.48/kg or $2480/tonne, based on the density of liquid N_2 (0.807 kg/L) from Al-Malah et al. (2018). CH_4 has a globally averaged unit price of $1.19/L (GlobalPetrolPrices, 2023), or $0.704/kg based on liquefied natural gas (LNG) (GOVUK, 2021). Therefore, to calculate the cost per kg of the SYNGAS feedstream, Eq.6 was applied:

$$\text{SYNGAS} = (N_2\,fraction \times Unit\ price\ of\ N_2) + (H_2\,fraction \times Unit\ price\ of\ H_2) + (CH_4\,fraction \times Unit\ price\ of\ CH_4)$$

$$\text{SYNGAS} = (0.737 \times 2.48) + (0.247 \times 1.6) + (0.0103 \times 0.704) = \$2.23/kg = \$2230/tonne\ (to\ nearest\ USD) \qquad (6)$$

$1.115/kg or $1115/tonne (June 2023) was assigned as the average unit cost of anhydrous NH_3 (USDA, 2023), to calculate the value of the PURGE stream from syngas (P_s) via Eq.7. In comparison, the unit price of grey NH_3 via LIQNH3 was \$1.607/kg or \$1607/tonne, as of April 2022 (Campion et al., 2023).

$$P_s = (N_2\ fraction \times Unit\ price\ of\ N_2) + (H_2\ fraction \times Unit\ price\ of\ H_2) + (NH_3\ fraction \times Unit\ price\ of\ NH_3) + (CH_4\ fraction \times Unit\ price\ of\ CH_4)$$

$$P_s = (0.223 \times 2.48) + (0.606 \times 1.6) + (0.028 \times 1.115) + (0.109 \times 0.704) = \$1.63/kg = \$1631/tonne\ (to\ nearest\ USD) \quad (7)$$

6.4.3.1.2 Equipment cost estimates

Base equipment costs were estimated by using the cost information via Arrarte (2022), that had been taken in May 2022 and adjusted to 2023. The estimated cost of MCOMP was an averaged cost from Arrarte (2022). An 8% inflation rate was assumed, before euro-to-USD conversion, based on findings from the Office for National Statistics (ONS) (ONS, 2023). USD was decided as the unit of currency, due to its prevalence throughout the literature. Table 6.5 presents a list of the equipment that had been used in Figure 6.2, as well as their corresponding estimated costs in USD.

Table 6.5 Equipment cost estimates for each component of the conventional model, adjusted to 2023 (Arrarte, 2022)

Equipment	Estimated cost (in USD)
MCOMP (Multi-stage compressor)	340,539.14
COMP2 (Single-stage compressor)	110,890.30
FSEP (Flash)	7,859.60
H1 (Direct heater)	138,454.76
H2 (Cooler)	1,028,420.98
RSTOIC (Reactor)	29,357.86

6.4.3.2 Clean

6.4.3.2.1 Stream data

In contrast to grey H_2, 'green' H_2 is generated via renewable electricity to power the PEM electrolysis stack. Production cost can range from €3-8/kg, depending on the region, according to PwC (2023) and IEA (2023). Desalination costs are relatively cheap and can range from \$0.5-1.5/L, depending on factors like electricity cost and plant size (Advisian, 2012; COSÍN, 2019; Smart Water Magazine, 2024). A production cost of €4/kg was decided for green H_2 generation, based on 2023 costs around the world. A mid-point of \$0.7/L was selected for the cost of seawater (H2OFEED) desalinisation.

$$€4/kg = \$4.29/kg = \$4290/tonne$$

$$\$1/L = \$1/kg = \$1000/tonne$$

The base cost for N_2 via a cryogenic ASU, that feeds into a NH_3 synthesis module, is provided by Thunder Said Energy (2023).

$$N_2 = \$20/ton = \$18/tonne \text{ (to nearest dollar)} = \$0.018/kg$$

Likewise, the cost and price of green (i.e. renewably-sourced) NH_3 vary greatly. Mid-points for cost and price were selected, based on the findings of Energy Technology Perspectives (IEA, 2023) and FuelCellsWorks (2022), respectively.

$$NH_3 \text{ price} = \$1.5/kg = \$1500/tonne$$

$$NH_3 \text{ cost} = \$964\text{-}1278/tonne = \$1121/tonne$$

The aforementioned stream data was applied for the cost of the clean PURGE stream, P_c, in the following calculation:

$$P_c = (N_2 \text{ fraction} \times N_2 \text{ via cryogenic ASU}) + (H_2 \text{ fraction} \times \text{green } H_2) + (NH_3 \text{ fraction} \times \text{green } NH_3)$$

And therefore:

$$P_c = (0.223 \times 0.018) + (0.610 \times 4.29) + (0.091 \times 1.121) = \$2.723/kg = \$2723/tonne \text{ (to nearest USD)}$$

6.4.3.2.2 Equipment cost estimates

Base equipment cost estimates for clean NH_3 had also been established from Arrarte (2022). The same 8% inflation rate was assumed, before euro-to-USD conversion, based on findings from the ONS (ONS, 2023). Both the N_2 and H_2 generation modules were identical to Arrarte (2022); therefore, the individual component costs were carried over in the cost estimations. However, the NH_3 synthesis module costs used in this case study had to deduct the cost of the shell-and-tube heat exchanger, in exchange for adding the costs of a single-stage compressor and a direct heater. Table 6.6 compares the NH_3 synthesis equipment used in the Aspen Plus flowsheet (Figure 6.6) with the equipment employed in the Arrarte's NH_3 synthesis module. Corresponding cost estimates are also included.

Table 6.6. Equipment cost estimates for each component of the NH_3 synthesis module, adjusted to 2023 (Arrarte, 2022)

Arrarte (2022)	Figure 6.6	Estimated cost in USD (Arrarte, 2022)	Estimated cost in USD (Figure 6.6)
C2 (Single-stage compressor)	CMP2 (Single)	110,890.30	110,890.30
C3 (Multi-stage compressor)	CMP3 (Multi)	340,605.57	340,605.57
C4 (Multi)	CMP4 (Multi)	340,472.70	340,472.70
X	CMP5 (Single)	X	110,988.88
REACTOR	REAC2 (Reactor)	29,357.86	29,357.86
F3 (Flash)	FS3 (Flash)	7,859.60	7,859.60
HX4 (Direct heater)	H3 (Direct)	155,628.40	155,628.40
HX5 (Heat exchanger)	H4 (Direct)	5,377.93	138,454.76
HX6 (Direct)	X	138,454.76	X
HX7 (Cooler)	H5 (Cooler)	1,028,420.98	1,028,420.98

6.5 Results

6.5.1 Stream data

Aspen Plus has a built-in emissions calculator. This was utilised to derive CO_2, CO, and CH_4 emissions data for each NH_3 production model (Table 6.7). Total cost flow estimates are shown in Tables 6.8-.9 for the conventional and clean NH_3 production models, respectively.

Table 6.7. GHG emissions for both models, based on the data from Aspen Plus

Greenhouse gas	Conventional (tonne/day)	Clean (tonne/day)
CO_2	17.97	0.00
CH_4	4.30	0.00
CO	0.26	0.00
Total	**22.53**	**0.00**

Table 6.8. Stream data for the conventional NH_3 synthesis module (Figure 6.2). *LIQNH3 has an output of 1330.3 tonne/day, with a unit price of $1607/tonne

Stream (total flowrate = 7000 kmol/hr)	Total cost flow in USD/day (to 2 d.p.)
SYNGAS	3.29×10^6
PURGE	233,343

*LIQNH3 (99.0% NH_3 purity)	1.48×10^6

Table 6.9. Stream data and process costs for the clean NH_3 production model (Figure 6.6)

Process/Stream	Mass flow in tonne/day (to 3 d.p.)	Total cost/value in USD/day (to 2 d.p.)
Desalinisation of H2OFEED	309.180 (H2OFEED)	309,180
Cryogenic air separation of AIRFEED	90.360 (AIRFEED)	1626.48
PURGE	8.497	934,688
Electrolysis of DESAL-1	302.297	1.30×10^6
NH3 (99.4% NH_3 purity)	72.652	8.99×10^7 (revenue)
	Total process cost (air separation, desalinisation, and electrolysis)	1.70×10^6

6.5.2 Total equipment cost estimates

Table 6.10 provides total cost equipment estimates for the equipment used in both conventional and clean NH_3 production models. It was assumed that equipment dimensions for Figure 6.3 were identical to those defined by Arrarte (2022).

Table 6.10. Equipment cost estimates for conventional and clean NH_3 production models

Equipment	Cost estimate in USD (c. May 2023)
Cryogenic ASU (2752.22 kg/h of 98.3% N_2)	23,053.36
PEM electrolyser (628.648 kg/h of 99.1 H_2)	576,204.30
NH_3 synthesis module (3027.15 kg/h of 99.3% NH_3)	2,262,679.05
Clean total (Figure 6.3)	**2,861,936.71**
Clean total (Arrarte, 2022)	**2,157,068.10**
Conventional total (Figure 6.2)	**1,655,522.64**

6.6 Socio-political perspectives

Truly holistically green sustainability must involve the successful, extensive, and in-depth implementation of the socio-political dimension(s) beyond solely worker safety (Guati-Rojo et al., 2021). Real, significant change towards holistically green and sustainable societies cannot occur when social and political (or socio-political) aspects are neglected or explored without depth, as is often the case in the literature (Lieder & Rashid, 2016; Geissdoerfer et al., 2017; Kirchherr et al., 2017). Socio-political drivers often play a major role in influencing other dimensions of green sustainability and vice versa. For example, the potential scalability and total costs of electrolyser technology of green H_2 generation for NH_3 production (Kurien & Mittal, 2022).

Moreover, socio-political attitudes and perceptions from general populace (and not just shareholders and industry executives) can significantly affect the implementation of green sustainability (Bronfman et al., 2012; Guati-Rojo et al., 2021; Kurien & Mittal, 2022). Due to a lack of data, Guati-Rojo et al. (2021) gathered data via a questionnaire on green NH_3 technology perceptions from Mexico and the UK, in addition to on a series of mostly close-ended questions (Table 6.11). Such questions had also asked about climate change and overpopulation perceptions, general attitudes towards pro-environmental action, and more.

Table 6.11. Questionnaire structure with the corresponding overall responses, based on Likert-scale answers. N=357 and N=563 for the UK and Mexico, respectively. *Political orientation is rated on a 0–10-point scale, with left-wing=0 and right-wing=10 (Guati-Rojo et al., 2021)

Questionnaire structure	Overall responses (Mexico/UK)
Demographics	Female = 56.8% / 67.2% Male = 42.8% / 30% Other = 0.4% (Mexico) / 2.8% (UK) 25-44 years old / 35-44 years old 53.6% have a university degree / 49.9% have a postgraduate degree Working full-time = 53.6% / 49.9% *Political orientation = 5.29 / 3.77
Climate change perceptions	**(‘Agree’ %; 1=not serious at all, 5=extremely serious)** Global climate is definitely changing? 95.7% / 88.7% Major concern? 68.2% / 60.9%

	Mainly driven by human activity? 81.4% / 84.1% Extreme threat for developing world? 70.1% / 61.4% National government is mainly responsible to act on the issue? 83.7% / 75.4% Industry is mainly responsible? 80.8% / 61.1%
Knowledge on climate change	Good baseline knowledge from citizens of both countries. However, Mexico has higher uncertainty on the exact causes of climate change Note: 29.7% / 38% answered that nuclear energy plants produce CO_2 emissions (they do not). An additional 33.6% / 32.8% answered "Don't know"
Perceptions on green NH_3 technologies	**With no prior information given, what immediately came to mind when thinking of NH_3** UK = smell (23.2%), manure/urine (15.1%), cleaning products (13.7%) Mexico = Poison/Toxic/Acid (25.2%), chemical (22.6%), cleaning products (16.5%) **After being told to read an excerpt on green NH_3, with emphasis on its 'greenness', their thoughts** Positive responses/perceptions = 87.7% / 82.9%
Green NH_3 deployment in their country	**Country implementation** Strongly support = 26.2% / 28.0% Support = 49.6% / 44.9% Strong opposition = 7.4% / 3.1% **Feasibility**

	Probably/Definitely = 36.9% / 64.1% Probably/Definitely NOT = 33.5% / 5.1% Unsure = 29.6% / 30.8% **Who is trusted to regulate?** UK = Government/Industry (43.8%) Mexico = Industry (44.6%)

The results demonstrated a mostly positive outlook on 'green' NH_3, despite an overall wariness of NH_3 as a chemical, as well as general support for the associated green technologies. However, said support was conditional to the perceived benefits and risks involved with implementation, as well as conditional on the trust in the institutions to regulate the green NH_3 technologies (Guati-Rojo et al., 2021). It is also apparent that, outside of green NH_3, there can be gaps in knowledge or even misinformation regarding climate change. If left unaddressed, this could have unforeseen impacts on the implementation of green NH_3 projects, that future research will be able to identify and evaluate in greater detail. The social/political/socio-political dimension(s) of green sustainability cannot be ignored with CPPs, such as green NH_3 production. Therefore, the proposed MCDM frameworks seek to address the gaps regarding holistically green and/or sustainable pathway prioritisation in small-scale CPPs, including but not limited to green NH_3 production.

6.7 Limitations

Although the clean model (Figure 6.3) did not generate GHG emissions, there could be indirect GHG emissions that were not considered. For example, GHG emissions via the transportation and storage of gaseous H_2 and N_2. If the electricity used for the production process is not (completely) renewable, this could also have significantly adverse effects on the potential viability and scalability of green NH_3, from a multi-dimensional perspective. Likewise, the conventional NH_3 synthesis module (Figure 6.2) did not consider the previous steps of the production process; namely, how the syngas feedstream (SYNGAS) had been produced, and/or how it was purified prior to the NH_3 synthesis module. However, it could be argued that this was outside of the system boundaries (and thus, scope of the project) in regard to this case study. The exact details and parameters of prior steps could have drastically affected various aspects within the scope of the case study to varied extents; production costs, product yields, etc.

Sensitivity analysis was also not applied for either NH_3 model. Sensitivity analysis is arguably essential in testing and evaluating the robustness of the NH_3 production models and/or its individual modules. This can be attributed to the limited capabilities of Aspen Plus v12.0 by itself, which also prevented the implementation of a more design-accurate and relatively cheaper shell-and-tube heat exchanger, in exchange for a director heater and conventional closed synthesis loop. Additionally, even if cost estimates could provide reasonable economic/financial outlines for both NH_3 models, there was a not-insignificant degree of uncertainty regarding cost estimates. It was also unclear as to how the scalability of both plant models could affect their capabilities, such as capacities and total costs. The degree of uncertainty could be attributed to a lack of access to reliable and accurate (techno-)economic analysis software. A lack of access to specialised techno-economic software was also why operational costs were not calculated in the process simulation. Additionally, costing and pricing can be greatly influenced on the contingent of various spatial-temporal and often multi-dimensional drivers; this includes seasonal variations in feedstock supply, local/regional/national socio-political factors, and transportation logistics (Osman et al., 2020; Chehade and Dincer, 2021; Salmon and Bañares-Alcántara, 2022). Therefore, the development of a green NH_3 production model can be on a relatively case-to-case basis, especially if it is designed to be optimised towards truly holistically green sustainability.

Section 6.6 covers the lack of in-depth literature on the social and political (and socio-political) dimensions of green NH_3 production, as well as how they can be linked and/or integrated multi-dimensionally. This has made it relatively difficult to ensure that a truly holistically green sustainability perspective has been sufficiently addressed and incorporated. Nevertheless, the questionnaire results (Table 6.11) of Guati-Rojo et al. (2021) did provide a solid foundation for developing the social/socio-political dimension of green NH_3 production. But an eclectic range and sufficient quantity of data would be required in further and more in-depth research, for a truly holistic approach towards green sustainability.

6.8 Conclusions

NH_3 is an essential component of our society. The H-B process is the main method of NH_3 production, particularly via a syngas feedstream composed of air-separated N_2 and SMR-derived H_2 gas. But, as society continues to grow and advance, our demand for NH_3 also increases. Therefore, in order to halt the degradation of our world, we must transition to greener and more sustainable means of NH_3 production ('green' NH_3). One of the most popular methods of producing green NH_3 is generating H_2 via PEM electrolysis and N_2 from a cryogenic ASU. Said method does not produce any GHG emissions, unlike SMR, though this is contingent on 100% renewable electricity. There was also a not-insignificant degree of uncertainty, particularly in regards to equipment cost estimates, albeit the exact degree cannot be unknown without reliable sensitivity analysis and up-to-date, specialised (e.g. Aspen) techno-economic analysis software. Additionally, because of the lack of access to specialised techno-economic analysis software, variables such as operational costs could not be considered in this project. Nevertheless, the methodologies and results can provide plenty of applicable information on NH_3 production (conventional and green). The project showed that scalability was possible for existing models with similar NH_3 outputs to small-scale plants (at a minimum). Moreover, while the socio-political dimension was severely lacking in regard to green NH_3 production, a solid foundation was still provided that can be further developed for truly holistically green NH_3 production.

Section 7.2 details a relatively simplistic FAHP model that was employed for small-scale, sustainable water desalination. Sections 7.3-.4 cover the development and implementation of a FAHP-TOPSIS for the prioritisation of holistically green and/or sustainable IPA and green NH_3 pathways. A relatively more complex and robust MCDM framework (FAHP-VIKOR with PROMETHEE-II) was proposed in section 7.5, to validate the methodology framework and provide a comparison of green NH_3 pathway rankings with FAHP-TOPSIS. Chapter 8 applies a small-scale bioethanol production case study to validate the final, (most) optimised methodology framework: the systematic integration of PSE tools (LCA, LCCA, and social-LCA) with FAHP-VIKOR & PROMETHEE-II.

7. Implementation of progressively more intricate, integrated MCDM frameworks

Section 3.3 outlines the project's overall MCDM methodology framework, to be integrated with PSE tools under WPD philosophy (Section C.4). This chapter aims to validate the implementation of the following, increasingly more complex, integrated MCDM frameworks: FAHP, FAHP-TOPSIS, and FAHP-VIKOR with PROMETHEE-II. Said MCDM frameworks aim to establish overall reliable, robust, and accurate pathway prioritisation, regardless of CPP case study, with an increasingly more explicit drive towards holistically green and/or sustainable pathway prioritisation. Three simulation-based case studies (sustainable water desalination, IPA synthesis, and green NH_3 production) were modelled to highlight the flexibility and adaptability of the integrated FAHP-TOPSIS framework. Table 7.1 shows the potential pathways that were identified for each case study via LCAs, as well as the applied MCDM framework(s).

Table 7.1. Potential green and/or sustainable pathways for IPA, green NH_3, and sustainable water desalination (in order of increasing MCDM complexity, top-to-bottom)

Case study	Potential pathways	MCDM framework
Sustainable water desalination (energy configuration; capacity)	A1. 100% diesel; 50 m^3/day A2. 75% diesel / 25% solar; 50 m^3/day A3. 60% -- / 40% --; 50 m^3/day A4. 100% diesel; 200 m^3/day A5. 75% -- / 25% --; 200 m^3/day A6. 60% -- / 40% --; 200 m^3/day A7. 100% diesel; 500 m^3/day A8. 75% -- / 25% --; 500 m^3/day A9. 60% -- / 40% --; 500 m^3/day A10. 100% diesel; 1000 m^3/day A11. 75% -- / 25% --; 1000 m^3/day A12. 60% -- / 40% --; 1000 m^3/day	FAHP
(Isopropanol) IPA synthesis	1. Direct Propylene Hydration (PH) 2. Propylene Indirect Hydration (IAH) 3. Acetone Hydrogenation (AH)	FAHP-TOPSIS
Green NH_3 production	1. Wind turbine electrolysis (WGEA) 2. Solar photovoltaic electrolysis (PVEA) 3. Hydropower electrolysis (HPEA) 4. Biomass gasification electrolysis (BGEA) 5. Nuclear high temperature electrolysis (NTEA)	FAHP-TOPSIS FAHP-VIKOR with PROMETHEE-II

7.1 Aim & Objectives

- Aim: Develop and implement an increasingly more complex MCDM framework (FAHP; FAHP-TOPSIS; FAHP-VIKOR with PROMETHEE-II) for each of the three simulation-based case studies
  - **Objective 1:** Apply "fuzzy" logic to criteria (first-level indicators) and sub-criteria (second-level indicators)
  - **Objective 2:** Calculate and apply the criteria and sub-criteria objective, subjective, and combination weights to derive the MCDM rankings of the pathways for each case study
  - **Objective 3:** Evaluate method robustness via sensitivity analysis. And if proven necessary, change the selected optimal pathway(s)

7.2 FAHP (Sustainable water desalination)

In Excel and MATLAB v24.1, FAHP was utilised to rank twelve potential pathways for relatively small-scale, modular sustainable water desalination (Table 7.1). A linguistic-based fuzzy pairwise comparison matrix was created to derive the criteria weightings in MATLAB v24.1, from the following criteria to encompass sustainability: C1—modularity, C2—sustainability, C3—standalone potential, C4—efficiency, and C5—cost (see Appendix Z for corresponding sub-criteria). The FAHP framework was modified from Clara Bartram's AHP analysis of sustainable water desalination in Oman (Bartram et al., 2023). FAHP included the capability of using linguistic "fuzzy" variables for non-numerical data in MCDM, as opposed to the standard AHP methodology, so long as they were converted into their corresponding TFNs (Eq.1; Table 7.2). The CR was calculated to be acceptable at 0.039<0.1 (Saaty, 1987; Vaidya & Kumar, 2006; Jamwal et al., 2021).

Table 7.2. Linguistic-based fuzzy comparison matrix of crisp AHP values and corresponding TFNs (Zhang et al., 2023)

Linguistic variable	Crisp value (AHP)	TFN	Reciprocal TFN
Equally important (E)	1	(1,1,1)	(1,1,1)
Weakly important (W)	2	(1/2,1,3/2)	(2/3,1,2)
Fairly -- (F)	3	(1,3/2,2)	(1/2,2/3,1)
Strongly -- (S)	4	(3/2,2,5/2)	(2/5,1/2,2/3)
Very strongly -- (V)	5	(2,5/2,3)	(1/3,2/5,1/2)
Extremely -- (EI)	6	(5/2,3,7/2)	(2/7,1/3,2/5)

7.2.1 Rankings

Local weights for each pathway were derived via a fuzzy pairwise comparison matrix as per each criterion in Excel (Table 7.3). Appendices AA-I to AA-V provides a full breakdown of the pairwise comparison matrix for each of the following criteria (C1-5): modularity, sustainability, standalone potential, efficiency, and cost. Criterion are either beneficial (+) or non-beneficial (-), in relation to the desired parameters for the pathways, e.g. beneficial=higher values for sustainability (C2) but lower values for cost (C5). Local criteria weights (Table 7.4) were multiplied by the local matrix weights to generate the global weights (Table 7.5). The sum of the global weights for each pathway determined its ranking, with a greater sum value denoting a higher ranking (Table 7.5).

Table 7.3. Summary of local weights of each pathway per criterion (to 3 s.f.). (+/-) denote whether the criterion is beneficial or non-beneficial

Local	C1(+)	C2(+)	C3(+)	C4(+)	C5(-)
A1	0.0865	0.114	0.112	0.139	0.0907
A2	0.116	0.135	0.128	0.139	0.160
A3	0.130	0.190	0.176	0.139	0.160
A4	0.0679	0.0474	0.0715	0.0403	0.0307
A5	0.105	0.087	0.0945	0.0403	0.0581
A6	0.140	0.106	0.134	0.0403	0.0863
A7	0.0578	0.0431	0.0347	0.0898	0.0343
A8	0.0650	0.0634	0.0586	0.0898	0.0570
A9	0.0977	0.0831	0.0724	0.0898	0.107
A10	0.0281	0.0221	0.0248	0.0642	0.0375
A11	0.0413	0.0405	0.0437	0.0642	0.0637
A12	0.0652	0.0680	0.0503	0.0642	0.114

Table 7.4. Local criteria weights (to 3 s.f.). (+/-) denote whether the criterion is beneficial or non-beneficial

Criteria	W
C1, modularity (+)	0.189
C2, sustainability (+)	0.187
C3, standalone potential (+)	0.197
C4, efficiency (+)	0.187
C5, cost (-)	0.239

Table 7.5. Sum totals of global weights (to 3 s.f.) and corresponding pathway rankings

Global	C1*W1	C2*W2	C3*W3	C4*W4	C5*W5	SUM	RANK
A1	0.0163	0.0214	0.0221	0.0260	0.0217	0.108	3
A2	0.0219	0.0253	0.0252	0.0260	0.0383	0.137	2
A3	0.0245	0.0355	0.0346	0.0260	0.0384	0.159	1
A4	0.0128	0.00887	0.0141	0.00754	0.00735	0.0507	11
A5	0.0198	0.0163	0.0186	0.00754	0.0139	0.0762	6
A6	0.0264	0.0199	0.0265	0.00754	0.0207	0.101	4
A7	0.0109	0.00807	0.00684	0.0168	0.00821	0.0509	10
A8	0.0123	0.0119	0.0116	0.0168	0.0136	0.0662	8
A9	0.0185	0.0156	0.0143	0.0168	0.0257	0.0908	5
A10	0.00531	0.00414	0.00489	0.0120	0.00898	0.0353	12
A11	0.00780	0.00758	0.00862	0.0120	0.0152	0.0513	9
A12	0.0123	0.0128	0.00992	0.0120	0.0272	0.0742	7

According to the FAHP results, pathways with a more balanced diesel-to-solar ratio are ranked higher than the diesel(-leaning) configurations. Solely in terms of energy configuration, 60-40 pathways were ranked the highest, followed by 75-25 and 100% diesel. The high ranking of A1 (3rd) could be attributed to its relatively lower energy and fuel consumption, which made a significantly positive contribution towards its criteria weightings (Appendix AA). Moreover, the hybridisation of diesel with solar PV (i.e., renewable energy) has been known to improve the sustainability, overall efficiency, and stand-alone potential in small-scale water delivery while also maintaining competitive costs (Gökçek, 2018; Jiang et al., 2022).

On the other hand, it can be argued that the economic dimension could have been over-represented and/or overweighted by decision-makers, due to potential biases and/or simply decision-based fatigue. However, while possible (Gökçek, 2018), this would be more explicitly evident on a real-world, case-to-case basis. Furthermore, only the smallest-scale plant capacity (50 m^3/day; A3>A2>A1) appears to be the most optimal, with the assignment of overall lower ranking to the larger plant capacities. Additionally, such an assignment of lower rankings appears to more disparate with increasing plant capacity. Larger/upscaled sustainable water desalination could potentially require modifications to the (overall) methodology framework, which is dependent on site-specific spatial and temporal variables, such as the brackish content (Belessiotis et al., 2016; Loutatidou et al., 2017; Mahmoudi et al., 2023) and/or available sunlight hours (Opricovic & Tzeng, 2007; Feroz et al., 2012).

Weighting issues (section B.3) could be one of the potential limitations of the AHP/FAHP and larger-scale methodology frameworks, which could be mitigated/removed by MCDM integration. The following sections integrate FAHP with TOPSIS (section 7.3-.4) and VIKOR with PROMETHEE-II (section 7.5), with more clearly defined social, economic, environmental, and technical criteria and corresponding sub-criteria. The following sections will ideally incorporate more balanced, holistically green and sustainable perspectives into the MCDM process for relatively small-scale CPPs.

7.3 FAHP-TOPSIS (IPA and Green NH_3)

The FAHP-TOPSIS framework was coded in MATLAB v24.1 by Zhaomin Li, MSc of Chemical Engineering, for the IPA synthesis via isopropyl acetate case study. FAHP (section B.3) enabled the use of both quantitative and qualitative data, in contrast to the standard AHP methodology, to derive (more) accurate and reliable criteria and sub-criteria weights for MCDM evaluation. In addition to its accessibility via MATLAB code, TOPSIS (section B.4) was integrated with FAHP to further enhance the robustness of the MCDM framework. FAHP-TOPSIS also utilises the high computational efficiency of TOPSIS to produce straightforward, reliable, and accurate pathway rankings; this is based upon the positive- and negative-ideal solutions, in relation to criteria and sub-criteria (Kumar et al., 2017; Balioti et al., 2018; Wu & Abdul-Nour, 2020; Al-Majali & Zobaa, 2025). TOPSIS can be summarised into the following steps (Balioti et al., 2018; Wu & Abdul-Nour, 2020):

1. Calculate the decision matrix, *A*; *m* = alternatives, with respect to *n* criteria; a_{ij} = intersection of each criterion and alternative [Eq.8]
2. Derive the normalised decision matrix, R, with the equation for $r_{ij.,}$ typically via vector normalisation (i = 1, 2, 3…, *m*; j = 1, 2, 3…, *n*) [Eq.9]
3. Calculate the weighted normalised matrix, *T* [Eq.10] via [Eq.11], where i = 1, 2, 3…, *m*; j = 1, 2, 3…, *n.* w_j = *j* criteria weighting
4. Determine the positive-ideal and negative-ideal solutions. Balioti et al. (2018) applies fuzzy logic, while the classical method applies crisp numbers [Eq.12 & Eq.13, respectively]
5. Calculate the distances of each alternative from the positive-ideal and negative-ideal solutions, D_i^+ and D_i^-, respectively [Eq.14 & Eq.15]
6. Derive relative closeness, C_i ; '1' = positive-ideal, '0' = negative-ideal [Eq.16]
7. Creating the preference ranking order; max C_i = the optimum alternative

$$A = (a_{ij})_{mn} \tag{8}$$

$$r_{ij} = \frac{a_{ij}}{\sqrt{\sum_{k=1}^{m} a_{kj}}^2} \tag{9}$$

$$T = (t_{ij})_{mn} \tag{10}$$

$$t_{ij} = r_{ij} * w_j \tag{11}$$

$$S^+ = \{\tilde{t}_1{}^+, \tilde{t}_2{}^+, \tilde{t}_n{}^+\} \tag{12}$$

$$S^- = \{\tilde{t}_1{}^-, \tilde{t}_2{}^-, \tilde{t}_n{}^-\} \tag{13}$$

$$D_i{}^+ = \sqrt{\sum_{j=1}^{n}}(t_{ij} - t_j{}^+)^2 \tag{14}$$

$$D_i{}^- = \sqrt{\sum_{j=1}^{n}}(t_{ij} - t_j{}^-)^2 \tag{15}$$

$$C_i = \frac{D_i{}^-}{(D_i{}^+ + D_i{}^-)} \tag{16}$$

A consistency level of ≤10% (CR≤0.1) is deemed acceptable (Karami, 2011; Prasad & Kousalya, 2017). To minimise potential information loss during weight aggregation (Cheng, 2004), the combined coefficient u=0.5 has been assigned where appropriate. It should also be noted that there is no single ideal method to deriving criteria (and sub-criteria) weights; the literature has varying methodologies that can be equally valid (Saaty, 1987; Xu et al., 2018; Olabanji & Mpofu, 2020), and thus can be dependent on a specific case-to-case basis.

7.3.1 Criteria and sub-criteria

The integrated FAHP-TOPSIS framework covered four key criteria regarding sustainable IPA and green NH_3 production: technical, economic, environmental, and social. Each criterion had three sub-criteria, that is illustrated below in Tables 7.6-.7. Three sub-criteria per criterion was decided as the appropriate number; too few sub-criteria would be unusable in the MATLAB model, while too many would have increased the likelihood of data distortion, including but not limited to rank reversal (Papathanasiou, 2021). As discussed throughout the review, there has been a lack of in-depth literature and social databases geared towards the social dimension(s) for holistically green sustainability, even in relatively current literature (Stojcic et al., 2019; Fonseca et al., 2021; Guati-Rojo et al., 2021; Kurien & Mittal, 2022). Therefore, the social (and by extension, the political) criteria had been expanded to include a greater number of social sub-criteria, and integrated into the MCDM framework with the other criteria. Said social sub-criteria were specialised to each case study beyond employee safety, based on literature findings (Bronfman et al., 2012; Guati-Rojo et al., 2021; Kurien & Mittal, 2022).

Table 7.6. Criteria and sub-criteria for IPA: technical (tech), economic (econ), environmental (env), and social (soc)

Tech (A)	Econ (B)	Env (C)	Soc (D)
A1: Conversion rate	B1: Total operational costs	C1: Human toxicity	D1: Intrinsic safety
A2: IPA selectivity	B2: Process complexity	C2: CO_2 emissions	D2: Policy relevance
A3: Tech maturity	B3: Total annual costs	C3: Pollution	D3: Public perception

Table 7.7. Criteria and sub-criteria for green NH_3 production: environmental (env), economic (econ), social (soc), and technical (tech)

Env (A)	Econ (B)	Soc (C)	Tech (D)
A1: Biodiversity loss	B1: Total operational costs	C1: Employer safety	D1: Exergy efficiency
A2: GHG emissions	B2: Sales prices	C2: Policy applicability	D2: Energy efficiency

A3: Global Warming Potential	B3: Net Present Value potential	C3: Public perception	D3: Green performance

7.3.2 Subjective weights

Like in section 7.2, FAHP was applied to enable the use of linguistic "fuzzy" variables for qualitative data in MCDM via conversion into their corresponding TFNs (Zhang et al., 2023). This was achieved via a relatively straightforward, linguistic-based fuzzy comparison matrix (Table 7.2). Fuzzy pairwise judgement matrices were established for the first layer index (Tables 7.8-.9) and sub-criteria of each criterion (Tables 7.10-.14), in order to later be able to derive the comprehensive subjective criteria weights, W_c, and combination weights, W_i. Said matrices were derived from individual and collaborative group evaluations among decision-makers. Because CR≤0.1 for all matrices, the consistency levels were deemed acceptable. Decision-makers were given temporal flexibility to carry out the evaluations, in order to prevent/minimise decision-making fatigue and stress, that could also introduce and/or exacerbate bias.

Table 7.8. First-layer (i.e., the criteria) subjective pairwise comparison matrix for IPA. REI, RV, and RF are the reciprocals of EI, V, and F, respectively

	A	B	C	D
A (Tech)	E	REI	RV	RF
B (Econ)		E	F	V
C (Env)			E	F
D (Soc)				E

Table 7.9. First-layer (i.e., the criteria) subjective pairwise comparison matrix for green NH_3 production

	A	B	C	D
A (Env)	E	REI	RV	RF
B (Econ)		E	F	V
C (Soc)			E	F
D (Tech)				E

Table 7.10. Fuzzy judgements converted into TFNs with the CR, subjective criteria weights (W_r), and fuzzy synthetic extent values, *S* (to 3 s.f.)

	A	B	C	D	CR	W_r	S
A	(1,1,1)	(2/7,1/3,2/5)	(1/3,2/5,1/2)	(1/2,2/3,1)	0.0186	0.122	0.0887

B	(5/2,3,7/2)	(1,1,1)	(1,3/2,2)	(2,5/2,3)		0.402	0.272
C	(2,5/2,3)	(1/2,2/3,1)	(1,1,1)	(1,3/2,2)		0.290	0.188
D	(1,3/2,2)	(1/3,2/5,1/2)	(1/2,2/3,1)	(1,1,1)		0.185	0.119

Table 7.11. Fuzzy judgement matrix for criteria A, where W_s = subjective sub-criteria weight (to 3 s.f.)

A	A1	A2	A3	CR	W_s	S		
A1	(1,1,1)	(3/2,2,5/2)	(1/2,2/3,1)	0.0873	0.372	0.247	0.373	0.570
A2	(2/5,1/2,2/3)	(1,1,1)	(1/2,2/3,1)		0.221	0.156	0.220	0.338
A3	(1,3/2,2)	(1,3/2,2)	(1,1,1)		0.408	0.247	0.407	0.633

Table 7.12. Fuzzy judgement matrix for criteria B (to 3 s.f.)

B	B1	B2	B3	CR	W_s	S		
B1	(1,1,1)	(3/2,1,2)	(1/2,2/3,1)	0.0566	0.4176	0.250	0.421	0.667
B2	(1/2,1,3/2)	(1,1,1)	(3/2,1,2)		0.249	0.167	0.246	0.208
B3	(1,3/2,2)	(1/2,1,3/2)	(1,1,1)		0.333	0.208	0.333	0.533

Table 7.13. Fuzzy judgement matrix for criteria C (to 3 s.f.)

C	C1	C2	C3	CR	W_s	S		
C1	(1,1,1)	(3/2,1,2)	(3/2,1,2)	0.0455	0.489	0.324	0.492	0.723
C2	(1/2,1,3/2)	(1,1,1)	(1/2,2/3,1)		0.296	0.195	0.295	0.442
C3	(1/2,1,3/2)	(1/2,2/3,1)	(1,1,1)		0.216	0.154	0.213	0.321

Table 7.14. Fuzzy judgement matrix for criteria D (to 3 s.f.)

D	D1	D2	D3	CR	W_s	S		
D1	(1,1,1)	(1,3/2,2)	(3/2,2,5/2)	0.0349	0.454	0.288	0.458	0.696
D2	(1/2,2/3,1)	(1,1,1)	(1,3/2,2)		0.325	0.206	0.322	0.506
D3	(2/5,1/2,2/3)	(1/2,2/3,1)	(1,1,1)		0.221	0.156	0.220	0.338

7.3.3 Objective weights

Before the objective weights could be derived, the data had to be normalised. This was because of the differences in scale among sub-criteria, as well as the varied units of measurement, that could cause severe data distortion. TOPSIS was therefore selected as the ranking method, with its ability to apply data normalisation via vector normalisation.

7.3.3.1 Data normalisation

The following equations were used for the positive indicators [Eq.17] and negative indicators [Eq.18]:

$$_{ij}(+) = \frac{f'_{ij} - \min(f'_{ij})}{(\max f'_{ij} - \min f'_{ij})}$$

(17)

$$f_{ij}(-) = \frac{\max(f'_{ij}) - f'_{ij}}{(\max f'_{ij} - \min f'_{ij})}$$

(18)

Where f_{ij} represents normalised data, and f'_{ij} represents original data for IPA and green NH_3 (Tables 7.15-.16, respectively). To ensure non-zero results for later logarithmic calculations, and avoid potential calculation errors, a constant *C* of 0.0001 was added to the normalised data (Tables 7.17-.18). *C*=+0.0001 was deemed sufficient to prevent data processing issues, while also being of negligible impact to the final results.

Table 7.15. Original "raw" data for the three IPA pathways per each sub-criterion (without units). '+' and '-' denote positive and negative indicators, respectively

	PH	AH	IAH
A1 (+)	0.85	0.7	0.96
A2 (+)	0.96	0.97	0.95
A3 (+)	9	9	8
B1 (-)	5.532	7.245	4.321
B2 (+)	1	2	2
B3 (-)	9.638	10.441	7.879
C1 (-)	349.65	199.025	98.762
C2 (-)	1476.302	2032.015	1073.3
C3 (+)	1	2	2
D1 (-)	30	25	20
D2(+)	1	1	2
D3(+)	2	1	0

Table 7.16. Original data for the five green NH_3 pathways per each sub-criterion (with units, if applicable)

	WGEA	PVEA	HPEA	BGEA	NTEA
A1, kg (-)	0.82	0.87	0.13	0.09	0.95
A2, kg CO_2 eq (-)	0.47	0.86	0.37	0.85	0.84
A3, 10^{-2} kg Sb eq (-)	0.35	0.63	0.29	0.28	0.64
B1, M$;(t/day) (-)	3.318	4.549	3.615	1.341	2.23
B2(+)	0.231	0.279	0.165	0.173	0.151

B3, % (+)	27.3	14	47.9	1.9	9
C1, scores (-)	16	16	16	33	49
C2(+)	0.267	0.267	0.234	0.149	0.084
C3(+)	0.247	0.211	0.289	0.126	0.126
D1, % (+)	16.4	9.4	42.7	15.4	23.8
D2(+)	0.204	0.179	0.234	0.179	0.204
D3(+)	0.179	0.179	0.33	0.202	0.11

Table 7.17. Normalised data for the IPA pathways (to 3 s.f.)

	Constant added +0.0001		
IPA pathway	PH	AH	IAH
A1 (+)	0.577	0.0001	1.00
A2 (+)	0.500	1.00	0.0001
A3 (+)	1.00	1.00	0.0001
B1 (-)	0.586	0.0001	1.00
B2 (+)	0.0001	1.00	1.00
B3 (-)	0.314	0.0001	1.00
C1 (-)	0.0001	0.600	1.00
C2 (-)	0.580	0.0001	1.00
C3 (+)	0.0001	1.00	1.00
D1 (-)	0.0001	0.500	1.00
D2(+)	0.0001	0.0001	1.00
D3(+)	1.00	0.500	0.0001

Table 7.18. Normalised data for the green NH_3 pathways (to 3 s.f.)

	Constant added +0.0001				
Low-carbon pathway	WGEA	PVEA	HPEA	BGEA	NTEA
A1, kg (-)	0.151	0.0931	0.954	1.00	0.0001
A2, kg CO_2 eq (-)	0.796	0.0001	1.00	0.0205	0.0409
A3, 10^{-2} kg Sb eq (-)	0.806	0.0279	0.972	1.0001	0.0001
B1, M$;(t/day) (-)	0.384	0.0001	0.291	1.0001	0.723
B2(+)	0.625	1.00	0.109	0.172	0.0001
B3, % (+)	0.552	0.263	1.00	0.0001	0.154

C1, scores (-)	1.00	1.00	1.00	0.485	0.0001
C2(+)	1.00	1.00	0.820	0.355	0.0001
C3(+)	0.742	0.522	1.00	0.0001	0.0001
D1, % (+)	0.210	0.0001	1.00	0.180	0.433
D2(+)	0.455	0.0001	1.00	0.0001	0.455
D3(+)	0.314	0.314	1.00	0.418	0.0001

7.3.3.2 Calculating W_o from entropy weighting

Entropy weighting was utilised to calculate the objective (sub-criteria) weights, W_o. The first step was to calculate the characteristic proportions, P_{ij} [Eq.19; Tables 7.19-.20], of each sub-criteria for each pathway.

$$P_{ij} = \frac{f_{ij}}{\sum_{i-1}^{n} f_{ij}} \tag{19}$$

Table 7.19. Characteristic proportion, P_{ij}, values for the IPA pathways (to 3 s.f.)

	A1	A2	A3	B1	B2	B3	C1	C2	C3	D1	D2	D3
PH	0.366	0.333	0.500	0.369	5.00E-05	0.239	6.25E-05	0.367	5.00E-05	6.67E-05	1.00E-04	0.667
AH	6.34E-05	0.667	0.500	6.30E-05	0.500	7.61E-05	0.375	6.33E-05	0.500	0.333	1.00E-04	0.333
IAH	0.634	6.67E-05	5.00E-05	0.631	0.500	0.761	0.625	0.633	0.500	0.667	1.00	6.67E-05

Table 7.20. P_{ij} values for the green NH_3 pathways (to 3 s.f.)

	A1	A2	A3	B1	B2	B3	C1	C2	C3	D1	D2	D3
WGEA	0.0688	0.429	0.287	0.160	0.328	0.280	0.287	0.315	0.328	0.115	0.238	0.153
PVEA	0.0424	5.38E-05	0.00993	4.17E-05	0.525	0.134	0.287	0.315	0.230	5.48E-05	5.24E-05	0.153
HPEA	0.434	0.538	0.347	0.121	0.0574	0.508	0.287	0.258	0.442	0.549	0.524	0.489
BGEA	0.455	0.0110	0.356	0.417	0.0902	5.08E-05	0.139	0.112	4.42E-05	0.0989	5.24E-05	0.204
NTEA	4.55E-05	0.0220	3.56E-05	0.301	5.24E-05	0.0784	2.87E-05	3.15E-05	4.42E-05	0.237	0.238	4.89E-05

Entropy value, e_j, and the coefficient of difference, g_j, of i-th object for each j-th (sub-)criterion were then derived using the following equations [Eq.20 and Eq.21, respectively]:

$$_{j} = -\frac{1}{\ln n}\Sigma_{i=1}^{n}\left(P_{ij}\ln P_{ij}\right)$$

(20)

$$g_j = 1 - e_j$$

(21)

$$W_o = \frac{g_j}{\Sigma_{j-1}^{m} g_j}$$

(22)

Where *n* is the number of pathways/routes; n=3 for IPA, and n=5 for green NH_3 production. Eq.22 was then applied to calculate W_o, where *m* is the total number of g_j values. Tables 7.21-.22 illustrate the calculation results for $P_{ij}\ln P_{ij}$ and their respective sum totals. Tables 7.23-.24 contains the results for e_j, g_j, and W_o.

Table 7.21. $P_{ij}\ln P_{ij}$ results for each sub-criterion and respective sum totals (Σ) for the IPA pathways (to 3 s.f.)

Sub-criterion	PH	AH	IAH	Σ
A1	-0.368	-0.000613	-0.289	-0.657
A2	-0.366	-0.270	-0.000641	-0.637
A3	-0.347	-0.347	-0.000495	-0.694
B1	-0.368	-0.000609	-0.291	-0.659
B2	-0.000495	-0.347	-0.347	-0.694
B3	-0.342	-0.000722	-0.208	-0.550
C1	-0.000605	-0.368	-0.294	-0.662
C2	-0.368	-0.000612	-0.289	-0.658
C3	-0.000495	-0.347	-0.347	-0.694
D1	-0.000641	-0.366	-0.270	-0.637
D2	-0.000921	-0.000921	-0.000200	-0.00204
D3	-0.270	-0.366	-0.000641	-0.637

Table 7.22. $P_{ij}\ln P_{ij}$ results for each sub-criterion and Σ for the green NH_3 pathways (to 3 s.f.)

Sub-criterion	WGEA	PVEA	HPEA	BGEA	NTEA	Σ
A1	-0.184	-0.134	-0.362	-0.358	-0.000455	-1.04
A2	-0.363	-0.000529	-0.333	-0.0497	-0.0840	-0.831
A3	-0.358	-0.0458	-0.367	-0.368	-0.000365	-1.14
B1	-0.293	-0.000421	-0.256	-0.365	-0.361	-1.28
B2	-0.366	-0.338	-0.164	-0.217	-0.000517	-1.09

B3	-0.357	-0.269	-0.344	-0.000502	-0.200	-1.17
C1	-0.358	-0.358	-0.358	-0.274	-0.000300	-1.35
C2	-0.364	-0.364	-0.350	-0.245	-0.000326	-1.32
C3	-0.366	-0.338	-0.361	-0.000443	-0.000443	-1.07
D1	-0.249	-0.000538	-0.329	-0.229	-0.341	-1.15
D2	-0.342	-0.000516	-0.339	-0.000516	-0.342	-1.02
D3	-0.288	-0.288	-0.350	-0.325	-0.000485	-1.25

Table 7.23. e_j, g_j, and W_o results for each sub-criterion for the IPA pathways (to 3 s.f.)

Sub-criterion	e_j	g_j	W_o
A1	0.598	0.402	0.0735
A2	0.580	0.420	0.0769
A3	0.631	0.369	0.0675
B1	0.600	0.400	0.0732
B2	0.631	0.369	0.0675
B3	0.501	0.499	0.0914
C1	0.603	0.397	0.0727
C2	0.599	0.401	0.0734
C3	0.631	0.369	0.0675
D1	0.580	0.420	0.0769
D2	0.00186	0.998	0.183
D3	0.580	0.420	0.0769
	SUM	5.46	

Table 7.24. e_j, g_j, and W_o results for each sub-criterion for the green NH_3 pathways (to 3 s.f.)

Sub-criterion	e_j	g_j	W_o
A1	0.646	0.354	0.102
A2	0.516	0.484	0.139
A3	0.708	0.292	0.0837
B1	0.793	0.207	0.0594
B2	0.675	0.325	0.0933
B3	0.727	0.273	0.0784
C1	0.838	0.162	0.0463
C2	0.822	0.178	0.0511
C3	0.662	0.338	0.0969
D1	0.714	0.286	0.0820
D2	0.636	0.364	0.104
D3	0.777	0.223	0.0640
	SUM	3.49	

7.3.4 Combination weights

W_c had to be calculated to derive W_i, in order to fully implement TOPSIS. W_i was calculated to encompass an overall weighting for each criterion and sub-criterion that combines objective and (comprehensive) subjective perspectives, while also mitigating/removing potential uncertainty with individual weights. Ideally, combination weights represent weightings from an overall holistically green and/or sustainable perspective. Eq.23 and Eq.24 were used to derive each set of weights, respectively, where u=0.5 (section 7). Tables 7.25-.26 show the results of the weight aggregation.

$$w_c = w_r w_s \tag{23}$$

$$w_i = \frac{(w_c)^u (w_o)^{1-u}}{\sum_{i=1}^{n} (w_c)^u (w_o)^{1-u}} \tag{24}$$

Table 7.25. All weight results by sub-criteria for the IPA pathways (to 3 s.f.)

Criteria	Sub-criteria	W_s	W_c	CR	W_o	W_i
A	A1	0.372	0.0455	0.0873	0.0735	0.0607
	A2	0.221	0.0270		0.0769	0.0479
	A3	0.407	0.0499		0.0675	0.0609
B	B1	0.418	0.168	0.0566	0.0732	0.116
	B2	0.249	0.100		0.0675	0.0863
	B3	0.333	0.134		0.0914	0.116
C	C1	0.489	0.142	0.0455	0.0727	0.107
	C2	0.296	0.0859		0.0734	0.0834
	C3	0.216	0.0626		0.0675	0.0683
D	D1	0.454	0.0839	0.0349	0.0769	0.0843
	D2	0.325	0.0601		0.183	0.110
	D3	0.221	0.0408		0.0769	0.0588

Table 7.26. All weight results by sub-criteria for the green NH_3 pathways (to 3 s.f.)

Criteria	Sub-criteria	W_s	W_c	CR	W_o	W_i
	A1	0.372	0.0455		0.102	0.0730

A	A2	0.221	0.0270	0.0873	0.139	0.0657
	A3	0.407	0.0499		0.0837	0.0694
B	B1	0.418	0.168	0.0566	0.0594	0.107
	B2	0.249	0.100		0.0933	0.104
	B3	0.333	0.134		0.0784	0.110
C	C1	0.489	0.142	0.0455	0.0463	0.0870
	C2	0.296	0.0859		0.0511	0.0711
	C3	0.216	0.0626		0.0969	0.0836
D	D1	0.454	0.0839	0.0349	0.0820	0.0890
	D2	0.325	0.0601		0.104	0.0851
	D3	0.221	0.0408		0.0640	0.0549

7.4 FAHP-TOPSIS rankings (IPA and Green NH_3)

TOPSIS (section B.4) was applied to rank the IPA and green NH_3 production pathways. Because the pathway data has already been normalised and transformed into P_{ij} (Tables 7.19-.20), further manual data processing was not required for the calculations in this section. Only the following sub-criteria weight types were used in the ranking calculations, to represent a relatively balanced weighting analysis, evaluation, and comparisons: W_o, W_c, and W_i. Said sub-criteria weights were agreed to encompass an overall holistically green and/or sustainable 'perspective' for each pathway, by creating an in-depth profile of how objectivity, (comprehensive) subjectivity, and/or the combination of both can affect criteria/sub-criteria. W_c was selected over W_s to consider the product subjectivity of criteria and sub-criteria. Each weight type could be analysed and evaluated individually, as well as compared to each other, to provide a clearer understanding of how each weighting type can/may influence the MCDM rankings.

7.4.1 Distances from ideal solutions

D_i^+ and D_i^- represent the distances from the positive (Eq.14) and negative (Eq.15) ideal solutions, respectively, with u=0.5. Lower D_i^+ values denote smaller deviations from the positive-ideal solutions; thereby, aligning closest with positive criteria/farthest from negative criteria, that denote the most optimal pathway(s) (Xu et al., 2018). Therefore, IAH and HPEA were regarded as the most optimal pathways for their respective case studies. Moreover, the use of individual and combination weights served to validate the pathway rankings via TOPSIS and suggests relatively high ranking stability, albeit this assumption did not consider the impacts of sensitivity analysis (section 7.6). Tables 7.27-.28 illustrate the distances for IPA and green NH_3 pathways, respectively.

Table 7.27. Distances from the positive- and negative-ideal solutions for each IPA pathway, based only on the combination, objective, and (comprehensive) subjective sub-criteria weights (to 3 s.f.)

	W_i		W_o		W_c	
	D_i^+	D_i^-	D_i^+	D_i^-	D_i^+	D_i^-
PH	0.532	0.298	0.573	0.307	0.504	0.286
AH	0.551	0.326	0.588	0.335	0.529	0.315
IAH	0.250	0.632	0.292	0.648	0.206	0.625

Table 7.28. Distances from the positive- and negative-ideal solutions for each green NH_3 pathway, based only on the combination, objective, and (comprehensive) subjective sub-criteria weights (to 3 s.f.)

	W_i		W_o		W_c	
	D_i^+	D_i^-	D_i^+	D_i^-	D_i^+	D_i^-
WGEA	0.244	0.267	0.247	0.280	0.235	0.259
PVEA	0.366	0.225	0.392	0.207	0.344	0.233
HPEA	0.180	0.404	0.161	0.431	0.192	0.375
BGEA	0.365	0.222	0.386	0.219	0.341	0.228
NTEA	0.388	0.142	0.411	0.128	0.364	0.156

7.4.2 Goodness-of-fit

Goodness-of-fit is the degree of fitness of each potential pathway to the D_i^- and D_i^+ values, in accordance with Eq.16. No significant deviations were apparent in the results of each weight type, which suggests relatively high stability. Moreover, goodness-of-fit for the D_i^+ (C_i^+) appears to be in-line with the pathway rankings for each case study. Subsequently, this has enhanced the reliability and accuracy of the rankings for decision-making. Tables 7.29-.30 show the goodness-of-fit, C_i^- and C_i^+, for each potential pathway in IPA and green NH_3 production, respectively.

Table 7.29. Goodness-of-fit for each IPA pathway, based only on the combination, objective, and comprehensive subjective sub-criteria weights (to 3 s.f.)

	W_i		W_o		W_c	
	C_i^-	C_i^+	C_i^-	C_i^+	C_i^-	C_i^+
PH	0.359	0.248	0.349	0.249	0.362	0.244
AH	0.371	0.257	0.363	0.259	0.373	0.251
IAH	0.716	0.495	0.689	0.492	0.752	0.506

Table 7.30. Goodness-of-fit for each green NH_3 pathway, based only on the combination, objective, and comprehensive subjective sub-criteria weights (to 3 s.f.)

	W_i		W_o		W_c	
	C_i^-	C_i^+	C_i^-	C_i^+	C_i^-	C_i^+
WGEA	0.522	0.233	0.531	0.241	0.525	0.229
PVEA	0.381	0.170	0.345	0.157	0.404	0.176
HPEA	0.692	0.309	0.728	0.330	0.662	0.289
BGEA	0.378	0.169	0.362	0.164	0.401	0.175
NTEA	0.268	0.120	0.238	0.108	0.299	0.131

7.5 FAHP-VIKOR with PROMETHEE-II (Green NH_3)

In contrast to TOPSIS, VIKOR (section B.6) utilises normalised values that are independent of the criterion's evaluation unit via linear normalisation (Opricovic & Tzeng, 2004; Opricovic & Tzeng, 2007). Furthermore, VIKOR can provide a more reliable representation of decision-maker viewpoints via compromise solutions with no/minimal data distortion (Opricovic & Tzeng, 2004). The steps of VIKOR are summarised below (Liu et al., 2014; Kannan et al., 2021; Papathanasiou, 2021; Vakilipour et al., 2021):

1. Establish the pairwise matrix per each alternative + evaluate criterion via linguistic assessments; i = 1, 2, 3… m; j = 1, 2, 3… n
2. Derive the average decision matrix, f_{ij}, where t = expert [Eq.25]
3. Calculate the best and worst values—f_j^+ and f_j^-, respectively—for criterion j [Eq.26 & Eq.27, respectively]
4. Derive the R_i and S_i values, where w_j = criteria weighting associated with relative importance [Eq.28 & Eq.29, respectively]. R_i = alternative i distance from negative-ideal; S_i = alternative i distance from positive-ideal
5. Work out Q_i [Eq.30], where v = weight associated with the application of the max group tool strategy. R^* = MinR_i; R^- = MaxR_i; S^* = MinS_i; S^- = MaxS_i
6. Evaluate the alternative rankings created from the Q_i values; lower value = higher ranking

$$f_{ij} = \frac{1}{k}\sum_{t=1}^{k} x_{ij}^{t} \tag{25}$$

$$f_j{}^{+} = max f_{ij} \tag{26}$$

$$f_j{}^{-} = min f_{ij} \tag{27}$$

$$R_i = MAX[w_j \frac{(f_j{}^{+} - f_{ij})}{(f_j{}^{+} - f_j{}^{-})}] \tag{28}$$

$$S_i = \sum_{j=1}^{n} w_j \frac{(f_j{}^{+} - f_{ij})}{(f_j{}^{+} - f_j{}^{-})} \tag{29}$$

$$Q_i = v\frac{(S_i - S^*)}{(S^- - S^*)} + (1-v)\frac{(R_i - R^*)}{(R^- - R^*)} \tag{30}$$

PROMETHEE-II was integrated with the FAHP-VIKOR framework, due to allowing decision-makers to carry out the complete ranking of alternatives, and its popular application in green sustainable research fields (Abedi et al., 2012; Cinelli et al., 2014; Jamwal et al., 2021). It has a relatively high level of stability and reliability, while also providing decisive results with/without grey data, and without the pre-requisite data normalisation (Brans et al., 1986; Gilliams et al., 2005; Wu & Abdul-Nour, 2020). FAHP provided the appropriate criteria and sub-criteria weightings via decision-makers, which mitigates one of PROMETHEE's key potential weaknesses (Behzadian et al., 2010; Kumar et al., 2017). PROMETHEE-II can be summarised into the following steps (Pohekar & Ramachandran, 2004; Abedi et al., 2012):

1. Create the evaluation matrix, in which alternatives will be compared from the basic data
2. Work out the difference in alternative performances, $d_j(a,b)$, where $g_j(a)$ and $g_j(b)$ are alternative performances for *a* and *b*, respectively in relation to criterion *j* [Eq.31]
3. Build and derive the preference functions [Gaussian, one of the six most common; Eq.32]. Decision-maker(s) may assign preference to an alternative that has been compared; preference functions are between 0 and 1 for each criterion. Add '-' for reversed alternative preference, i.e. b>a. $P_j(a,b)$ = preference of *a* over *b*
4. Establish the q, p, and s parameters (or at least, two of the three, depending on the preference function); indifference, preference, and the Gaussian threshold, respectively
5. Calculate the aggregated preference indices per alternative pairs; w_j = weighting for criterion *j* [Eq.33]
6. Work out the outranking flows per alternative *a* and the other (n-1) alternatives; positive and negative [Eq.34 and Eq.35, respectively]
7. Derive the net outranking flows [Eq.36 for alternative *a*]
8. Obtain the complete alternative rankings in descending order

$$d_j(a,b) = g_j(a) - g_j(b) \tag{31}$$

$$P_j(a,b) = (\pm)F[d_j(a,b)] \tag{32}$$

$$\pi(a,b) = \sum_{j=1}^{k} P_j(a,b) * w_j \quad \forall a,b \in A \tag{33}$$

$$\varphi^+(a) = \frac{1}{n-1}\sum_{x \in A} \pi(a,x) \tag{34}$$

$$\varphi^{-}(a) = \frac{1}{n-1} \sum_{x \in A} \pi(x, a) \quad (35)$$

$$\varphi(a) = \varphi^{+}(a) - \varphi^{-}(a) \quad (36)$$

FAHP-VIKOR with PROMETHEE-II used the criteria and sub-criteria established in Section 7.3.1, as well as the weights from sections 7.3.2-.3.4, for the green NH_3 production case study. Section 7.5.1 displays and compares the rankings of each potential pathway via TOPSIS, VIKOR, and PROMETHEE-II.

7.5.1 Ranking comparisons

Tables 7.31-.33 compare the ranking metrics (top) and resultant rankings (bottom) of green NH_3 production via VIKOR and PROMETHEE-II, with the results obtained from TOPSIS (section 7.4). In terms of W_i (Table 7.31), HPEA is the overall most optimal pathway for green NH_3 production, albeit VIKOR offered WGEA as a possible compromise solution, in which either pathway would be considered the most optimal for decision-makers. There is contention between the overall prioritisation of PVEA and BGEA, in which the implementation of VIKOR and PROMETHEE-II were not clarified. However, NTEA can be regarded, with greater certainty, as the overall least optimal pathway for green NH_3 production when considering W_i.

Only the rankings based on W_o (Table 7.32) have shown consistency regardless of the MCDM ranking method. In contrast, W_c-based rankings (Table 7.33) appear to vary the most depending on the applied ranking method, albeit not to a significant degree.

Table 7.31. Comparison of TOPSIS, VIKOR, and PROMETHEE-II ranking metrics (top) and resultant rankings (bottom) for W_i (to 3 s.f.) *Compromise solutions

W_i	TOPSIS (D_P)	VIKOR (Q_i)	PROMETHEE-II ($\varphi(a)$)
WGEA (1)	0.244	0.257	0.152
PVEA (2)	0.366	0.965	-0.133
HPEA (3)	0.180	0.279	0.442
BGEA (4)	0.365	0.984	-0.105
NTEA (5)	0.388	0.984	-0.356

Rankings	TOPSIS	VIKOR	PROMETHEE-II
WGEA (1)	2	1*	2
PVEA (2)	3 or 4	3	4
HPEA (3)	1	2*	1

BGEA (4)	3 or 4	4	3
NTEA (5)	5	4	5

Table 7.32. Comparison of TOPSIS, VIKOR, and PROMETHEE-II ranking metrics (top) and resultant rankings (bottom) for W_o (to 3 s.f.)

W_o	TOPSIS (D_P)	VIKOR (Q_i)	PROMETHEE-II ($\varphi(a)$)
WGEA (1)	0.247	0.229	0.164
PVEA (2)	0.392	0.895	-0.199
HPEA (3)	0.161	0.0001	0.523
BGEA (4)	0.386	0.833	-0.118
NTEA (5)	0.411	0.949	-0.371

Rankings	TOPSIS	VIKOR	PROMETHEE-II
WGEA (1)	2	2*	2
PVEA (2)	4	4	4
HPEA (3)	1	1*	1
BGEA (4)	3	3	3
NTEA (5)	5	5	5

Table 7.33. Comparison of TOPSIS, VIKOR, and PROMETHEE-II ranking metrics (top) and resultant rankings (bottom) for W_c (to 3 s.f.)

W_c	TOPSIS (D_P)	VIKOR (Q_i)	PROMETHEE-II ($\varphi(a)$)
WGEA (1)	0.235	0.151	0.150
PVEA (2)	0.344	0.817	-0.0829
HPEA (3)	0.192	0.121	0.363
BGEA (4)	0.341	0.555	-0.0866
NTEA (5)	0.364	0.797	-0.344

Rankings	TOPSIS	VIKOR	PROMETHEE-II
WGEA (1)	2	2*	2
PVEA (2)	4	5	3
HPEA (3)	1	1*	1
BGEA (4)	3	3	4
NTEA (5)	5	4	5

7.6 Sensitivity analysis

As it was uncommon in the examined literature but highly recommended (chapter 2), sensitivity analysis was thus carried out to evaluate the overall robustness of each MCDM framework. Criterion weight (A-D) was altered at +0.1 increments, from +0 to +0.9, to produce a total of 40 variations with respect to the calculated C_i^+ (FAHP-TOPSIS, section 7.6.1), Q_i (FAHP-VIKOR, section 7.6.2), and $\varphi(a)$ (PROMETHEE-II; section 7.6.3) values. A total of 40 variations was decided as a good compromise between efficiency and efficacy.

7.6.1 FAHP-TOPSIS

Figures 7.1-.2 plot the sensitivity of C_i^+ relative to changes in weight for each criterion, A-D, for IPA and green NH_3 pathways, respectively. For each of the four key sustainability criteria, C_i^+ was relatively stable to alterations in criteria weight. A full breakdown of the sensitivity results for each criterion are tabulated in Appendices AB-AC for IPA and green NH_3 pathways, respectively.

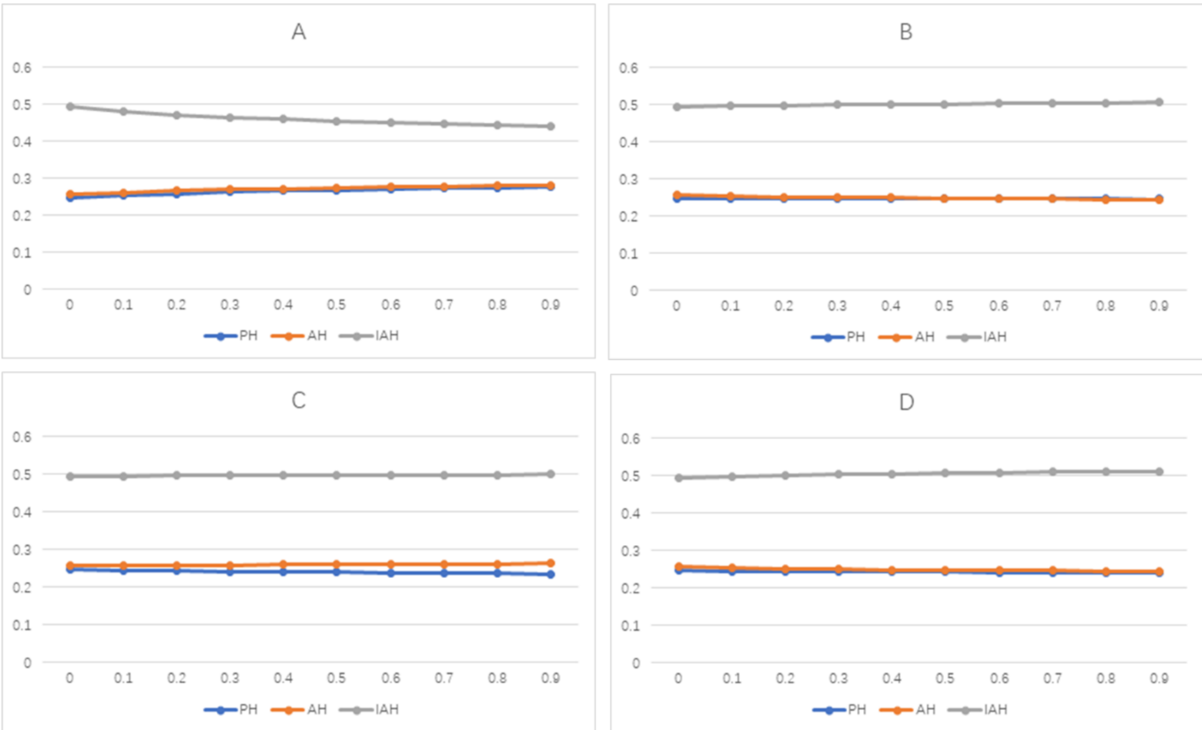

Figure 7.1. ***C_i^+*** **results relative to changes in technical (A; top-left), economic (B; top-right), environmental (C; bottom-left), and social (D; bottom-right) criterion weights for IPA pathways**

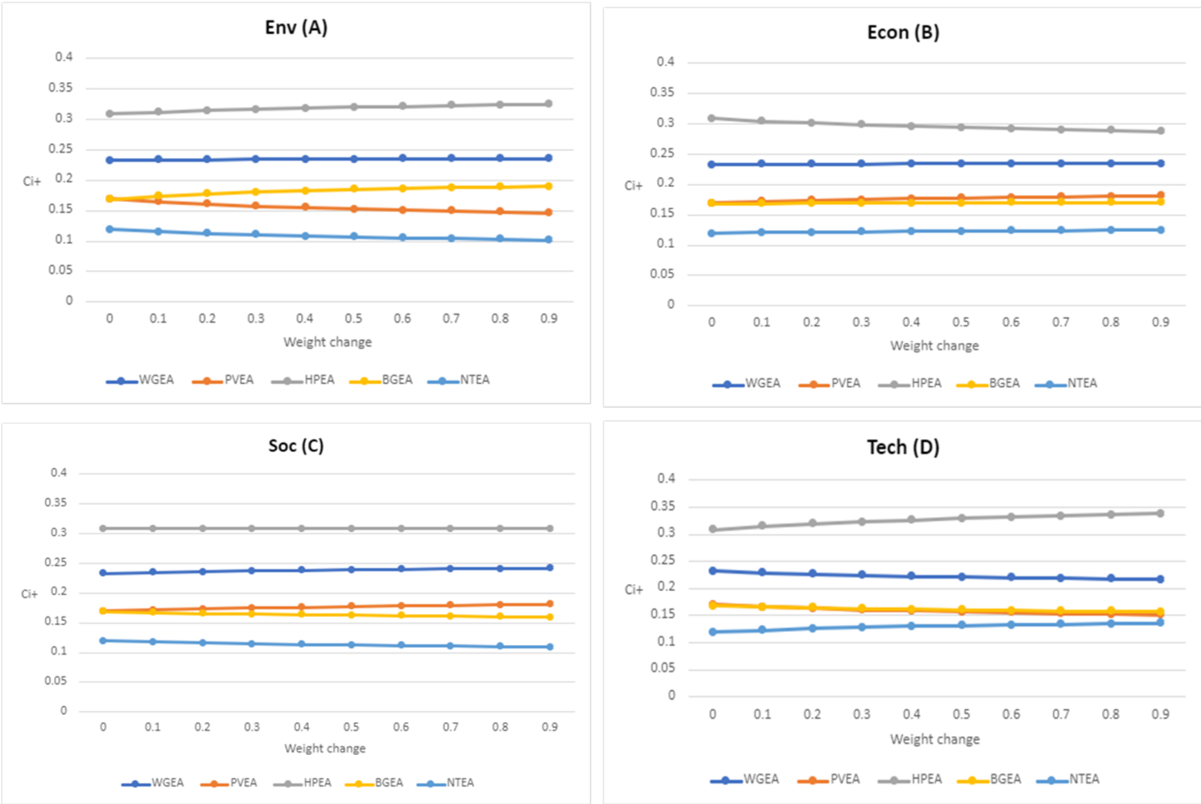

Figure 7.2. C_i^+ **results relative to changes in environmental (A; top-left), economic (B; top-right), social (C; bottom-left), and technical (D; bottom-right) criterion weights for green** NH_3 **pathways**

7.6.2 FAHP-VIKOR

Figure 7.3 plots the sensitivity of Q_i (based on W_i) relative to changes in weight for each criterion, A-D, for green NH_3 production pathways. Unlike Figures 7.1-.2, alterations in criteria weight seem to have had a much more explicit effect on Q_i values and consequently VIKOR stability, excluding the economic criteria (B). The resultant changes to Q_i also appeared to have affected the pathway rankings. This could have been due to various potential factors, such as criteria over-/under-weighting or the number of sub-criteria. However, without further research, it is currently unclear as to what exactly caused the instabilities in VIKOR.

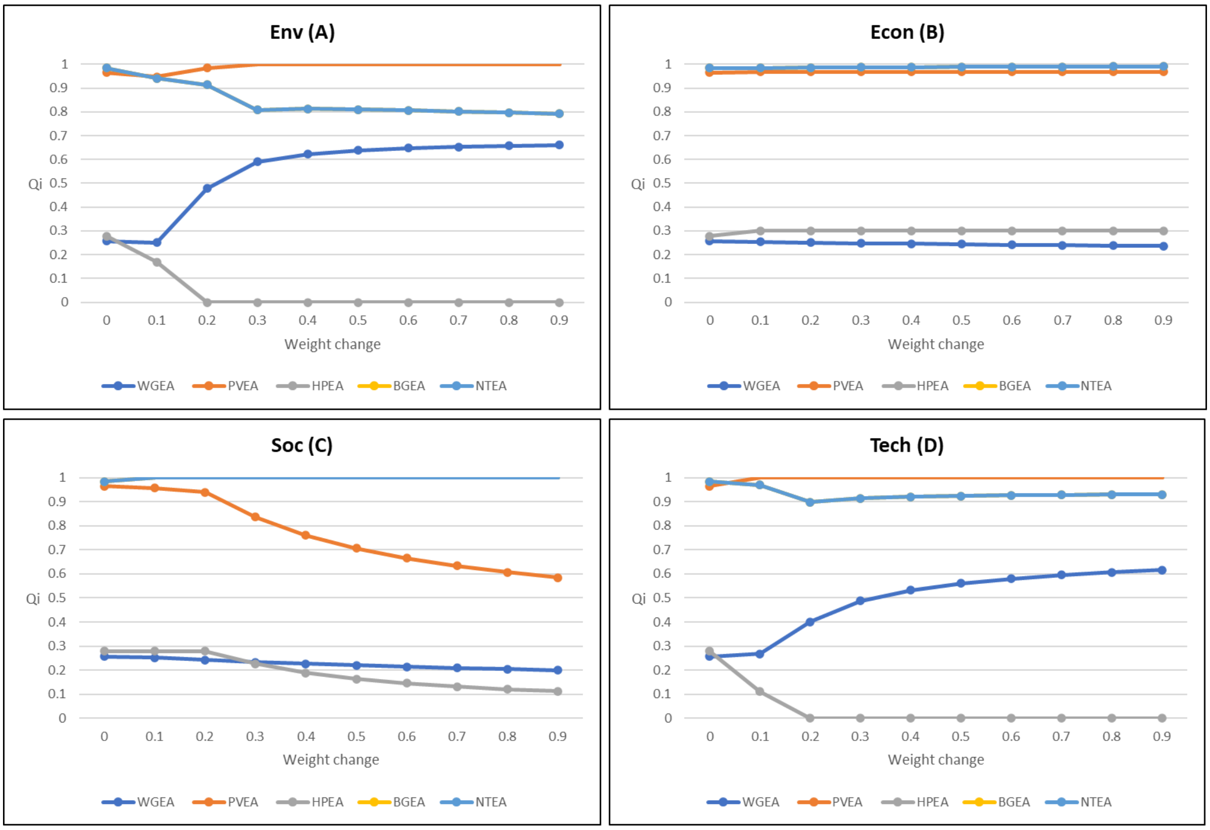

Figure 7.3. ***Q_i*** **results relative to changes in environmental (A; top-left), economic (B; top-right), social (C; bottom-left), and technical (D; bottom-right) criterion weights for the green NH_3 pathways. When** ***Q_i*****=1.0001, e.g. PVEA in Tech, the line is barely within the graph**

7.6.3 PROMETHEE-II

Figure 7.4 plots the sensitivity of *φ(a)* (based on W_i) relative to changes in weight for each criterion, A-D, for the green NH_3 production pathways. *φ(a)* appeared to be highly stable with incremental (+0.1) changes to criteria weights, particularly in contrast to VIKOR. PROMETHEE-II is well-documented as a highly stable and reliable ranking method. This can be attributed to its methodology (section B.7), in which the preference function and use of net outranking flows create less sensitivity to permutations relative to other MCDM methodologies (Brans et al., 1986; Gilliams et al., 2005; Wu & Abdul-Nour, 2020).

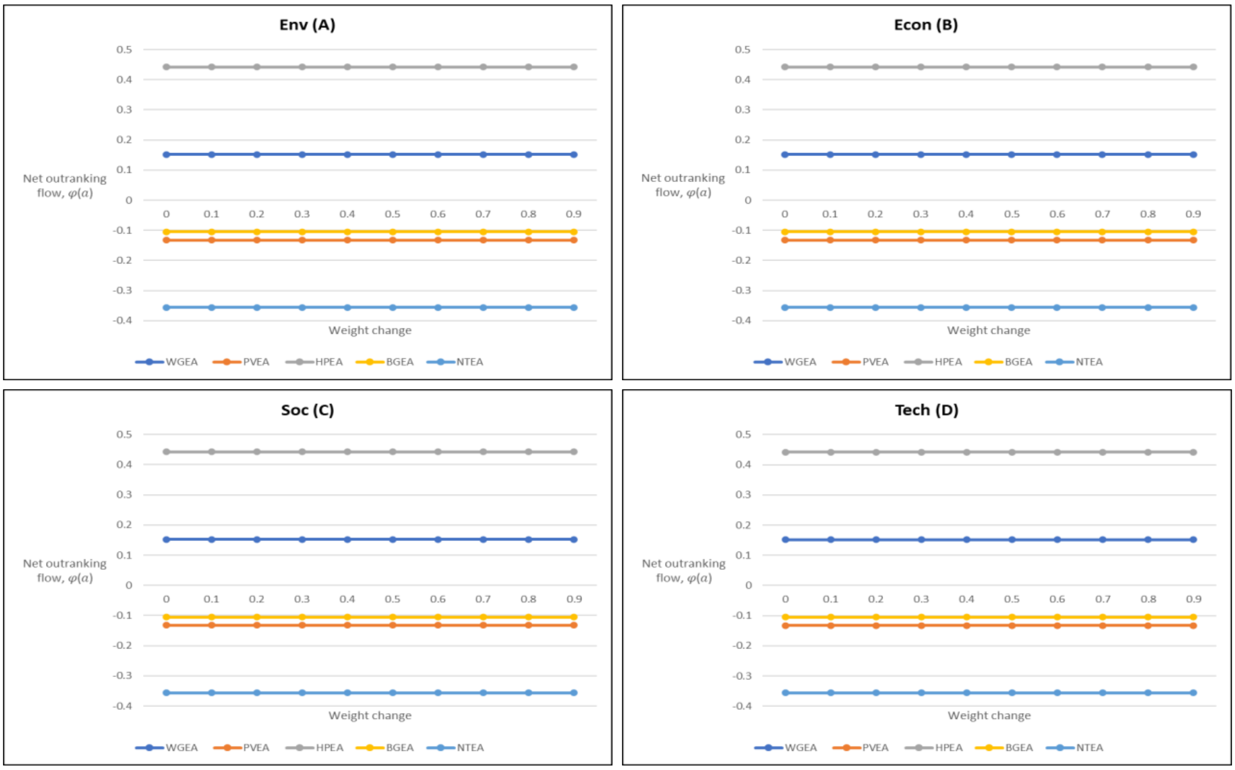

Figure 7.4. *φ(a)* results relative to changes in environmental (A; top-left), economic (B; top-right), social (C; bottom-left), and technical (D; bottom-right) criterion weights for green NH_3 pathways

7.7 Conclusions

FAHP was utilised to rank twelve potential diesel-solar energy configuration and plant capacity pathways for sustainable water desalination. The results determined that a greater incorporation of solar power is optimal, particularly at the smallest-scale capacity (50 m^3/day). On the other hand, there may be overweighting/over-representation of the economic dimension, that may have skewed rankings. FAHP-TOPSIS and FAHP-VIKOR with PROMETHEE-II serve to validate the implementation of integrated MCDM frameworks for prioritising (ideally) holistically green and/or sustainable IPA and NH_3 production pathways. However, data must be clearly processed (sections 7.3.3.1-.2) to maximise the understanding and effectiveness of the said integrated MCDM frameworks. According to the D_i^+ and C_i^+ values (Tables 7.27-.28), the most-to-least optimal pathway rankings for IPA is IAH>PH>AH, albeit there might be slight contention over the prioritisation of PH and AH, as well as BGEA and PVEA. Meanwhile, the most-to-least optimal pathways for green NH_3 production is HPEA>WGEA>BGEA/PVEA>NTEA, albeit the addition of VIKOR and PROMETHEE-II sowed contention among the middle rankings. Only W_o was consistent in rankings across methods.

Sensitivity analysis per criterion for IPA and green NH_3 (Figures 7.1-.3, 7.4) showed negligible changes in C_i^+ and *φ(a)* relative to weight change in +0.1 increments. On the other hand, while the C_i^+ values for W_i align with the above order of pathway prioritisation, VIKOR (Figure 7.3) showed notable instability with incremental weight change. Nevertheless, Figures 7.2-.4 show an overall stability in the MCDM results for each case study. There may be uncertainties among sub-criteria by themselves and in relation to each other, especially in terms of potential changes over time; exact equipment costs, NPV, and the specific social perceptions regarding the case studies. This can also make it difficult to ascertain the exact extent of which each sustainability dimension can affect pathway rankings, and to prioritise pathways per dimension. Among other considerations, that are further elaborated in section 9.1, future work must identify and address these uncertainties.

8. Experimental validation case study

8.1 Introduction

Biofuels have gained significant interest as sustainable alternatives to conventional fossil-fuels, particularly when derived from renewable feedstocks (Qiao et al., 2022; Senthil et al., 2022; Guimarães et al., 2023; Ye et al., 2024). Such renewable feedstocks can range from various animal wastes to crop residues, e.g. palm oil empty fruit bunch (EFB) (Srinophakun & Suwajittanont, 2022). Biofuels, such as bioethanol and biodiesel, can be green(er) fuel alternatives with lower overall GHG emissions and independence from fossil fuels (Alam & Tanveer, 2020; Guimarães et al., 2023; Mansy et al., 2024). Additionally, biofuels have various multi-dimensional potential benefits, such as addressing MSW (section A.5.2), and the potential for social development (Qiao et al., 2022). On the other hand, biofuel production can also have negative multi-dimensional impacts, if it is unsustainable in its life-cycle activities; land-use, transportation, storage, etc. (Silalertruksa & Gheewala, 2011). Furthermore, for biofuel production to be a long-term viable replacement to fossil fuels, it must address sustainability from a holistically green perspective; i.e., competitive feasibility and economic value (Alam & Tanveer, 2020; Mousavi-Avval et al., 2023), (socio-)political influences and impacts, and technological considerations (Alam & Tanveer, 2020). Holistically green and sustainable biofuel production could be one of the key potential pathways towards sustainable CEs (i.e., circular bioeconomies) (Rebolledo-Leiva et al., 2023), if sustainability is addressed from a holistically green perspective.

Bioethanol is one of the most popular liquid biofuels with significant potential as a sustainable, renewable energy resource (Halder et al., 2019; Alam & Tanveer, 2020; Qiao et al., 2022; Guimarães et al., 2023). Consequently, its demand as an alternative fuel is likely to continue rapidly increasing over the next few decades, particularly with increasing global energy demands (Silalertruksa & Gheewala, 2011; Halder et al., 2019; Qiao et al., 2022). Therefore, bioethanol production was chosen as a case study for holistically green sustainability in CPPs. Raw (potato) starch was selected as renewable feedstock for the "pilot-scale" (i.e., scale of a pilot plant), experiment-based bioethanol case study. Potatoes are starch-rich, inexpensive, ubiquitous on a global-scale, and a high biomass-producing (starch-to-sugar yields for fermentation) crop of high energy efficiency (Liu & Lien, 2016; Taha et al., 2019; Kumar et al., 2024). Moreover, potato waste (peels, pulp, process water, etc.) is highly abundant and starch-rich (Suresh et al., 2020). Therefore, potato waste can also serve as a viable (renewable) feedstock for bioethanol production, while simultaneously addressing MSW issues (section A.5), and promoting sustainable resource management (Taha et al., 2019; Suresh et al., 2020; Kumar et al., 2024). In terms of practicality, potato starch was also the most readily accessible feedstock. Sections 8.3-.5 elaborate on the experimental background, materials, and methods of the case study. This case study sought to validate the project's final, optimised methodology framework: the systematic integration of PSE tools (section 8.6) for better-defined sub-criteria selection, with the FAHP-VIKOR & PROMETHEE-II framework (section 8.7) and sensitivity analysis (section 8.8).

8.2 Aims & Objectives

- Aim 1: Integrate PSE tools with FAHP-VIKOR & PROMETHEE-II to create a final, optimised methodology framework
  - **Objective 1:** Create product portfolios for the bioethanol via Process Systems Engineering (PSE) tools: Life Cycle Assessment (LCA), Life Cycle Cost Analysis (LCCA), and Social-LCA
  - **Objective 2:** Identify the three key sustainability indicators per criteria; e.g., environmental=global warming potential, economic=NPV, etc.
  - **Objective 3:** Establish the three key sub-criteria per the four established criteria via the sustainability indicators, to be integrated into the final, optimised MCDM framework

- Aim 2: Apply the bioethanol case study to the final, optimised MCDM framework
  - **Objective 1:** Apply fuzzy-logic to criteria and sub-criteria
  - **Objective 2:** Calculate and apply the criteria and sub-criteria objective, subjective, and combination weights to derive the MCDM rankings of the bioethanol experimental runs (R1-3)
  - **Objective 3:** Evaluate method robustness via sensitivity analysis; if proven necessary, change the selected best alternative(s)

8.3 Background

To truly validate the systematic integration of the final and most optimised MCDM framework with PSE tools, the application of data from a non-simulation-based (i.e., experiment-based) case study was required. Thus, a series of three pilot plant, gate-to-gate bioethanol production experimental runs was conducted. The aim of this experiment was to distil ethanol via a mixture of raw potato starch and water, after liquefaction, saccharification, and fermentation [Eq.37].

$$C_6H_{12}O_6 + 2ADP + 2P_i \rightarrow 2C_2H_5OH + 2CO_2 + 2ATP \tag{37}$$

Glucose ($C_6H_{12}O_6$) from the mash–ground grains broken down into sugars, mixed in with water and heated–reacts with yeast (ADP=adenosine diphosphate; Pi=phosphate) to produce adenosine triphosphate (ATP), ethanol (C_2H_5OH), and carbon dioxide (CO_2). During the fermentation stage, aerobic metabolism is the preferred method of energy production via yeast (38:1 ATP-to-glucose moles), albeit this produces an undesired product: acetic acid. Therefore, the fermentation tank (B2) must be rendered airtight to force anaerobic metabolism.

8.4 Materials

Raw potato starch, α-amylase, γ-amylase, and antifoaming agent with water were mixed to form a slurry, a thick suspension of solids in liquid, that would be fermented in the fermentation tank. 0.1 M sulfuric acid and caustic soda (B3 and B4, respectively) were also added, as a means of pH regulation, while steam via a steam generator was utilised for cleaning purposes. A distillation unit (GUNT CE640e) was used to thermally distil ethanol from the fermented slurry. The GUNT CE640e unit consisted of the following key parts (Figure 8.1): mash tank (B1), fermentation tank (B2), and distillation tower (D1).

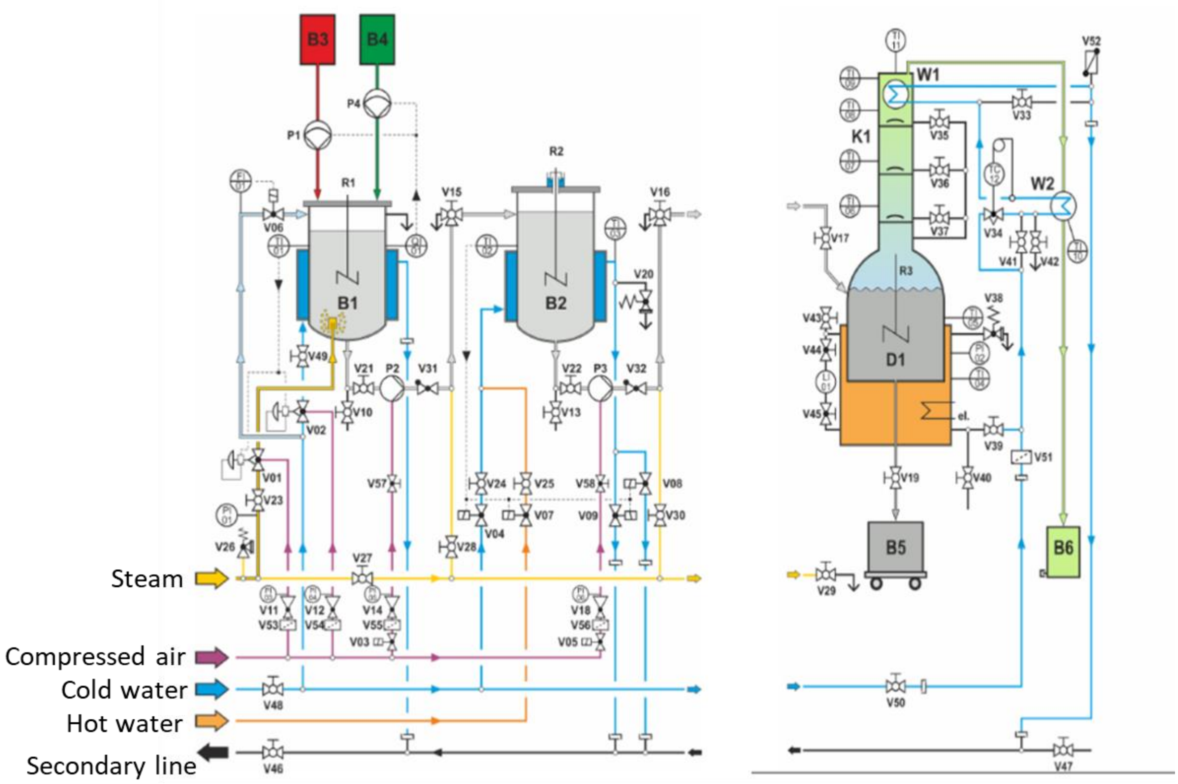

Figure 8.1. CE640e distillation unit: V-*n*=Valves, P-*n*=Pumps, B1=Mash tank, B2=Fermentation tank, B3=Acid tank, B4=Caustic solution tank, B5=Stillage tank, B6=Raw ethanol tank, W1=Dephlegmator, W2=Tube cooler, D1=Still, K1=Distillate column, R1-3=Stirrers

8.5 Methods

8.5.1 Safety

Prior to operation, all relevant valves were set to their correct positions. No contact was made with B1 nor the steam piping while in use, due to the risk of scalding. Pumps P2 and P3 were isolated during operation of the steam generator, as direct steam contact would have destroyed the pumps. The produced ethanol was appropriately stored away as per regulations, away from any potential ignition sources.

8.5.2 Step 1: Liquefaction

The purpose of liquefaction was to produce a sugar solution of di-, tri-, and oligosaccharides. Table 8.1 shows the valve positions for liquefaction and saccharification, which had to be done prior to unit operation. Firstly, a slurry of 1.5 kg of raw potato starch and 2 L of water was prepared without lumps. Once ready, 30 L of water was added to B1, followed by ~10% of the slurry mass.

Table 8.1. Liquefaction and saccharification valve positions

Valve	Position / Function	Valve	Position / Function	Valve	Position / Function
V01	Control valve	V21	closed	V41	closed
V02	Control valve	V22	closed	V42	closed
V03	Solenoid valve	V23	closed	V43	closed
V04	Solenoid valve	V24	open	V44	open
V05	Solenoid valve	V25	open	V45	open
V06	Solenoid valve	V26	Safety valve	V46	open
V07	Solenoid valve	V27	closed	V47	open
V08	Solenoid valve	V28	closed	V48	open
V09	Solenoid valve	V29	closed	V49	open
V10	closed	V30	closed	V50	closed
V11	Set pressure P_3 to 2 bar	V31	Non-return valve	V51	Strainer
V12	Set pressure P_4 to 2 bar	V32	Non-return valve	V52	Aerator
V13	closed	V33	closed	V53	Strainer
V14	Set pressure P_5 to 0.3 bar	V34	Control valve	V54	Strainer
V15	To outlet	V35	open	V55	Strainer
V16	To D1	V36	open	V56	Strainer
V17	closed	V37	open	V57	open
V18	Set pressure P_6 to 0.3 bar	V38	Safety valve	V58	open
V19	closed	V39	closed		
V20	Safety valve	V40	closed		

After dosing the mixture with α-amylase (0.3/1.15/2 mL) for the entire raw material mass, slurry was poured into B1 until the level reached the pH sensor. Shut-off valve V23 was then slowly opened. Temperature control in the programmable logic controller (PLC) was activated, and the on-screen reference variable *w* was set to 95°C. The stirrer speed for R1 was set to 50/min, while the on-screen pH reference variable *w* was set to 5.6. Upon reaching the set temperature, the mash was stirred for 30 minutes, before changing the temperature and pH to 56°C and 5.0, respectively. The temperature reduction is achieved via automatic closing of the steam control valve (V01) and opening of the cooling water valve (V02). Liquefaction was deemed complete upon reaching the new PLC reference variables.

8.5.3 Step 2: Saccharification

Saccharification decomposed the di-, tri-, and oligosaccharides into glucose (i.e. monosaccharide) only, ready for the fermentation stage. The first step was to add γ-amylase (5/10.5/16 gms) into B1. At least 30-45 mins had to pass, in which the temperature in B1 was 56°C. PLC reference variable *w* for the temperature control was then changed to 30°C, and the PLC pH control was deactivated. Once the new temperature was reached, the temperature control was also deactivated. Unfortunately, due to the equipment unavailability at the time, the glucose concentration of the saccharified product could not be tested.

8.5.4 Step 3: Fermentation

Fermentation converts glucose into ethanol via yeast in the absence of oxygen, i.e. anaerobic metabolism. Prior to this step, the following valves had to be appropriately adjusted (Table 8.2), the fermentation cap must be sufficiently filled, and B2 must be airtight to prevent aerobic fermentation. Moreover, the mash had to be transferred from B1 to B2 via pump P2 with the PLC. The three-way ball valve (V15) was set in the position of the drain line to hydraulically separate B2 from P2 and B1 to be later cleaned.

Table 8.2. Fermentation valve positions

Valve	Position / Function	Valve	Position / Function	Valve	Position / Function
V01	Control valve	V21	open	V41	closed
V02	Control valve	V22	closed	V42	closed
V03	Solenoid valve	V23	closed	V43	closed
V04	Solenoid valve	V24	open	V44	open
V05	Solenoid valve	V25	open	V45	open
V06	Solenoid valve	V26	Safety valve	V46	open
V07	Solenoid valve	V27	closed	V47	open
V08	Solenoid valve	V28	closed	V48	open
V09	Solenoid valve	V29	closed	V49	open
V10	closed	V30	closed	V50	closed
V11	Set pressure P_3 to 2 bar	V31	Non-return valve	V51	Strainer
V12	Set pressure P_4 to 2 bar	V32	Non-return valve	V52	Aerator
V13	closed	V33	closed	V53	Strainer
V14	Set pressure P_5 to 0.3 bar	V34	Control valve	V54	Strainer
V15	To B2	V35	open	V55	Strainer
V16	To D1	V36	open	V56	Strainer
V17	closed	V37	open	V57	open
V18	Set pressure P_6 to 0.3 bar	V38	Safety valve	V58	open
V19	closed	V39	closed		
V20	Safety valve	V40	closed		

B2 was dosed with ~6.67 gms of yeast, followed by 1.2 mL of anti-foaming agent via the filler hole that was then closed. B2 was equipped with stirrer R2; this was used to assure good, continuous mixing of the yeast and mash during fermentation. But in order to prevent increased foaming when using R2 (at 85/min), an automatic mode with an 'on time' and 'pause time" was calibrated at 1 min and 9 mins, respectively. Subsequently, the PLC reference variable *w* for the temperature control of B2 was set to 30°C. Fermentation required continuous temperature maintenance via supply of the following during the experimental runs: hot water, cold water, and electricity. Fermentation proceeded for approximately 72 hours, with completion indicated by the cessation of CO_2 bubbles from within the fermentation cap (or longer, in the case of run 3 at 192 hours). Due to faults with the heating system at the time, a makeshift heating pad set-up was employed to sustain the required fermentation temperature for B2.

8.5.5 Step 4: Clean-up

B1 and V15 had to be cleaned immediately upon starting the fermentation process; this was to prevent the mash residues from undergoing undesirable biological decomposition. B1 was cleaned via cold process water/steam, with prior assurance that B1 was properly connected to the drain line through P2 via V15. P2 and section of the main line were cleaned via remnant liquid from steam cleaning into the drain line via V15. Upon completion of cleaning, steam and compressed air supplies were switched off.

Immediately after distillation had started, B2 and the main line leading up to V16 also had to be cleaned with clean water via filler hole, to prevent undesirable biological decomposition. And so long as the water was relatively clean, it was then used to clean pump P3 via opening V22. If dirty, it was drained out via V19. The inside of the distillation unit itself was later cleaned with water.

8.5.6 Step 5: Distillation

Prior to fractional discontinuous rectification of ethanol, the following valves had to be appropriately adjusted (Table 8.3). The water bath of still D1 was then filled to level (above the red mark), with aid from the measuring point LI01. This was done with cold water via opening the V39 and V43 shut-off valves. Next, the PLC was used to transfer the contents of B2 into the distillation unit (Figure 8.2) via P3, as well as activate stirrer R3. As illustrated in Figure 8.3, a raw ethanol tank B6 was placed underneath the outlet of the raw ethanol reservoir.

Table 8.3. Distillation valve positions. NOTE: Due to not being used, V21 did not need to be opened, but V22 had to be opened

Valve	Position / Function	Valve	Position / Function	Valve	Position / Function
V01	Control valve	V21	open	V41	closed
V02	Control valve	V22	closed	V42	closed
V03	Solenoid valve	V23	closed	V43	closed
V04	Solenoid valve	V24	closed	V44	open
V05	Solenoid valve	V25	closed	V45	open
V06	Solenoid valve	V26	Safety valve	V46	open
V07	Solenoid valve	V27	closed	V47	open
V08	Solenoid valve	V28	closed	V48	open
V09	Solenoid valve	V29	closed	V49	closed
V10	closed	V30	closed	V50	open
V11	Set pressure P_3 to 2 bar	V31	Non-return valve	V51	Strainer
V12	Set pressure P_4 to 2 bar	V32	Non-return valve	V52	Aerator
V13	closed	V33	closed	V53	Strainer
V14	Set pressure P_5 to 0.3 bar	V34	set to 2	V54	Strainer
V15	To B2	V35	open	V55	Strainer
V16	To D1	V36	open	V56	Strainer
V17	open	V37	open	V57	open
V18	Set pressure P_6 to 0.3 bar	V38	Safety valve	V58	open
V19	closed	V39	closed		
V20	Safety valve	V40	closed		

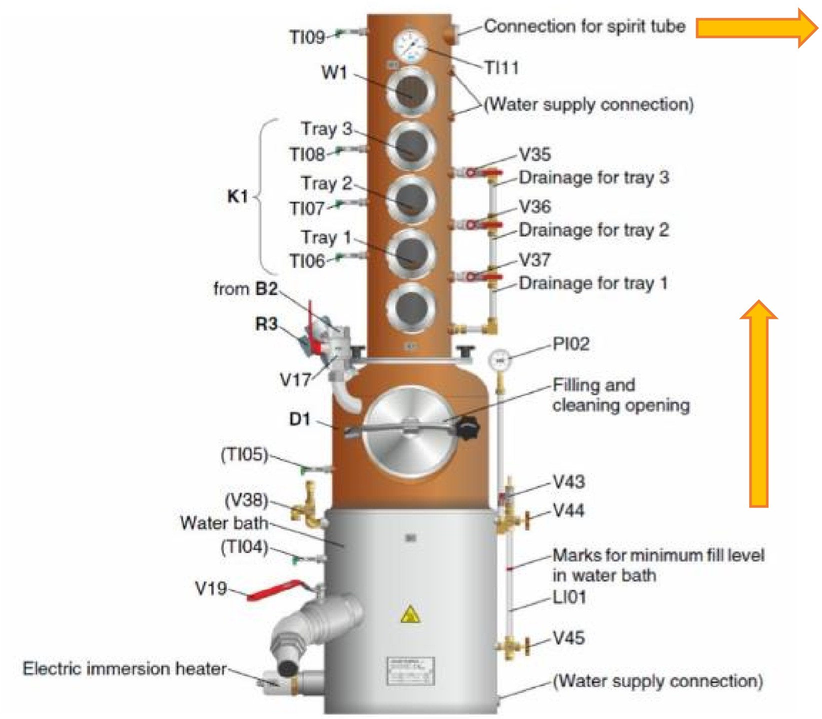

Figure 8.2. Distillation unit; three bubble cap trays without reflux (i.e., without heating of a chemical reaction for a specific amount of time, while continuously cooling the produced vapour back into a liquid via condenser) + separation stage with internal reflux. Distillation was controlled with the measured temperature (i.e. 'spirit temperature') above the dephlegmator (W1)

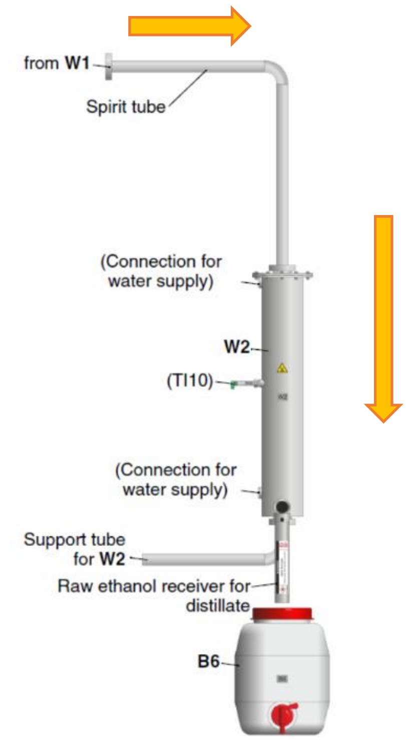

Figure 8.3. Flow of distillate into B6 for collection via spirit tube connection in Figure 8.2; W2=Tube cooler

The PLC's temperature control reference variable *w* was subsequently set to 78-79ºC (based on TI09), and V35-37 were closed. Heat for the distillation process was provided by an electrical heater in the water bath via PLC, while the dephlegmator (W1) and tube cooler (W2) were kept cold via cold water supply. Because of the initially insufficient amount of distillate, temperature *w* was gradually increased to 95ºC at 3ºC intervals. However, the distillation temperature was prevented from exceeding 98ºC. Once no further distillate could be collected, the heater was switched off. Ethanol content of the distillate, in terms of %purity, was then calculated using two of its variables, that were cross-referenced with a series of alcohol-to-water tables: temperature and density. Said variables were measured via an electronic thermometer and hydrometer, respectively.

8.6 Application of PSE tools

Section 3.4 proposed the implementation of a FAHP-VIKOR & PROMETHEE-II framework integrated with PSE tools (LCA, LCCA, and social-LCA), to derive the key sustainability sub-criteria; environmentally, economically, and socially, respectively. The systematic integration of PSE tools aims to further refine the MCDM methodology framework, into a comprehensive sustainability governance platform. Bioethanol production was selected as the experimental validation case study for the final, optimised methodology framework. Three experimental production runs (R1-3) were carried out with the CE640e distillation unit. Table 8.4 presents the collected raw data from R1-3 that was utilised by the PSE tools, in conjunction with the works of Ren et al. (2015) and Srinophakun & Suwajittanont (2022). Section 8.6.1-.6.3 elaborates on the methodology for each PSE tool that was utilised in this project.

Table 8.4. Raw data of the bioethanol production case study

Raw data	α_amylase (mL)	y_amylase (gms)	Purity (%)	Distilled (mL)	Days fermented
R1	0.3	5	60	90	3
R2	2	16	68	450	3
R3	1.15	10.5	46	434	8

8.6.1 LCA

LCA is a commonly used PSE tool that assesses a product's life cycle, in the context of (potential) environmental impacts; this includes raw resource acquisition, waste management, and the effects on human health and society (Dreyer et al., 2006; Finnveden et al., 2009; Goedkoop et al., 2016). Resultantly, LCA plays a prominent role in sustainability decision-making, from environmental policy to individual projects, as environmental awareness has become increasingly more important (Finnveden et al., 2009; Goedkoop et al., 2016; Rebolledo-Leiva et al., 2023). LCA was employed via the latest version of SimaPro (v9.6.0.1, as of writing), under ISO standards (14040 and 14044), in the context of a pilot-scale, experiment-based bioethanol production case study. Said case study involved three experimental runs (R1-3) with α-amylase and glucoamylase contents as the dependent variables. It should also be noted that the goals and scope of the project had to be amenable to optimisation-based adjustments (Goedkoop et al., 2016).

8.6.1.1 Goals & Scope

The project's LCA sought to identify the midpoint environmental impact categories of life-cycle activities from the pilot-scale bioethanol production case study, from a conglomeration of decision-maker backgrounds (researchers, industry professionals, amateurs, etc.). The overarching goal of the project was to provide a holistically green and/or sustainable perspective to various CPP case studies via MCDM, which was further enforced by the utilisation of LCA, LCCA, and social-LCA. LCA was employed to examine, assess, and define the environmental dimension of bioethanol production. Only the three most significant (environmental) sustainability factors were incorporated into the MCDM (FAHP-VIKOR & PROMETHEE-II) framework as the environmental sub-criteria.

8.6.1.2 Functional unit(s)

A 'functional unit' can be defined as the product(s)/service(s) to be assessed via PSE tools (Dreyer et al., 2006; Jørgensen et al., 2008). Project portfolios were created via the PSE tools; LCA, LCCA, and social-LCA. The functional unit was the same across the three PSE tools: bioethanol product in kilograms (kg). This served to link LCA, LCCA, and social-LCA to represent an overall holistic and integrated product portfolio for bioethanol production; environmentally, economically, and socially, respectively.

8.6.1.3 Inventory analysis

Input impact categories (Table 8.5) and output flows (Figure 8.4) were selected and identified, respectively, by utilising the in-built library databases of SimaPro v9.6.0.1; Ecoinvent 3 (system and unit), Agri-footprint–economic (system and unit), Industry data 2.0, and Methods. EU-Denmark Input Output Database was not included to emphasise the adaptable (i.e. non-case-specific) applicability of the project methodology, and to avoid a niche Euro-centric perspective. Process contribution analysis was also able to provide information on the relative contribution of each process, and therefore allowed the decision-makers to determine the most significant sustainability factors to implement into the final, optimised MCDM framework.

Table 8.5. Raw material inputs in LCA. Base*=the original experimental quantities in R1-3 (bioethanol, kg=0.042; 0.2417; 0.1577)

Input/Raw material	CAS-number	Base* quantity (kg)
Process water	007732-18-5	30
Sulfuric acid	007664-93-9	0.0098
Sodium hydroxide	001310-73-2	0.004
Potato starch	009005-25-8	1.5
α-amylase	009000-90-2	$3.75*10^{-7}$ (R1); $2.5*10^{-6}$ (R2); $1.44*10^{-6}$ (R3)
Glucoamylase	009032-08-0	$9.46*10^{-7}$ (R1); $3.03*10^{-6}$ (R2); $1.99*10^{-6}$ (R3)

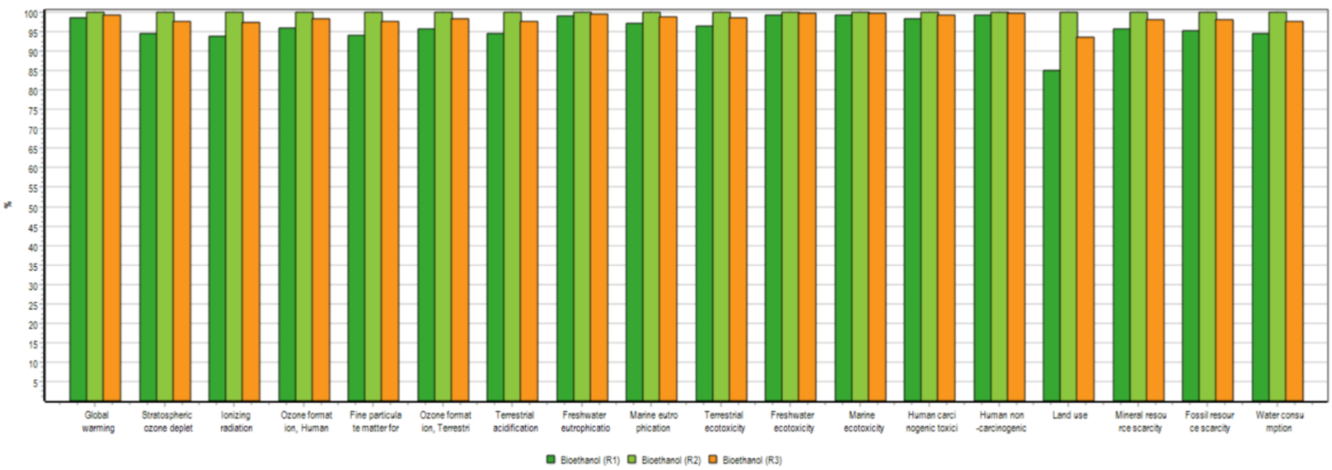

Figure 8.4. Characterisation comparisons of bioethanol production R1-3 per environmental impact category via LCA

8.6.1.4 System boundaries

ReCiPe 2016 Midpoint (H) v1.09 was employed to derive the most accurate and reliable representative of environmental impact categories for bioethanol production. Because the project scope was only focused on the 'feedstock conversion to ethanol' (sections 8.5.2-.6), the proposed system boundaries were limited to that of gate-to-gate analysis, as outlined in

Figure 8.5. Hierarchical (H) was selected over Individualist (I) and/or Egalitarian (E), as the former is a compromise between short-term optimism (I) and overly cautious, long-term planning (E) (Pré, 2016). A hierarchical perspective also provides overall less ambiguous environmental effects, on more global and long(er)-lasting scales (Huijbregts et al., 2017).

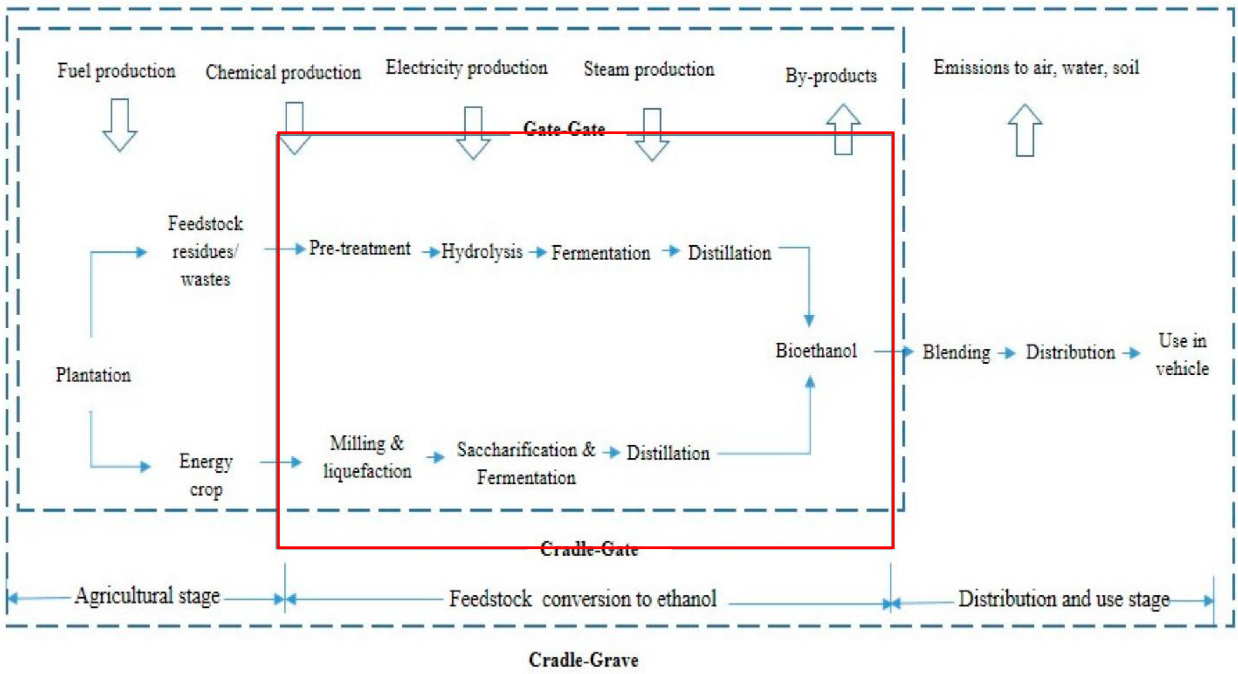

Figure 8.5. System boundaries for bioethanol production, from cradle-to-grave to gate-to-gate analysis. The project case study was limited to gate-to-gate; its system boundaries are outlined in red (Soleymani et al., 2021)

As explained in section 3.3.3, the key sub-criteria were defined based on the relative significance of each impact category, collaborative decision-maker discussions, and in accordance to the ISO 14044 standard. Only three key sustainability factors were selected based on the system boundaries (Figure 8.5), and the three most significant environmental impacts in relation to bioethanol production via ReCiPe 2016 and the literature (Junjie et al., 2012; Soleymani et al., 2021; Shakelly et al., 2023; Yin et al., 2024). Table 8.6 lists the environmental sub-criteria: human non-carcinogenic toxicity (non-c tox), terrestrial toxicity (terr tox), and global warming (GW).

Table 8.6. Environmental sub-criteria of the final, optimised MCDM framework via LCA in SimaPro

	Human non-c tox (kg 1,4-DCB)	Terr tox (kg 1,4-DCB)	GW (kg CO_2 eq)

R1	255	82.1	20.8
R2	257	85	21.1
R3	257	83.8	21

8.6.2 LCCA

LCCA can be defined as a decision-making methodology that analyses and assesses the life cycle of a product in terms of its economic variables, such as short-term and/or long-term cost-effectiveness (Li et al., 2019; Pernetti et al., 2021; Kumari et al., 2022). Like LCA, LCCA has found prominent usage in sustainability-related decision-making, as businesses—or more specifically, its stakeholders—view the economic dimension of sustainability with great importance (Awasthi et al., 2017; Li et al., 2019). This project employed LCCA, to be integrated with LCA and social-LCA, for a more holistic approach towards green sustainability in pilot-scale bioethanol production. As ISO 14040 and 14044 cannot be directly applied to LCCA, LCCA had be carried out under adapted forms of the aforementioned standards. Moreover, in order to avoid or mitigate the potential limitations of LCCA (Pernetti et al., 2021), the LCCA for this project: a) had to have clear, concise system boundaries and assumptions (see section 8.6.2.4); b) had to be capable of covering analysis over various spatial-temporal scales; c) had sufficiently accurate, reliable, and plentiful data, without being too difficult to collect/analyse; d) taken into account techno-economic aspects, such as annual operating expenses (OPEX).

8.6.2.1 Goals & Scope

The LCCA had to identify, understand, and evaluate the economic impact categories resulting from the life-cycle activities of the bioethanol production case study. Like the LCA, decision-maker backgrounds were varied to provide a more well-rounded decision-making process. LCCA was employed to examine, assess, and define the economic dimension of the case study. The economic impact categories also incorporated a technical dimension, with OPEX and total capital expenditure (CAPEX) estimates based on Srinophakun & Suwajittanont (2022). Only the three most significant sustainability factors were incorporated into the final, optimised MCDM framework as the economic sub-criteria.

8.6.2.2 Functional unit(s)

The functional unit was the same across the three PSE tools: bioethanol, kg.

8.6.2.3 Inventory analysis

Economic data estimates were based on bioethanol production via palm oil EFB in Srinophakun & Suwajittanont (2022), as opposed to potato starch in R1-3. Input impact categories (Table 8.7) and output flows (Figure 8.6) were selected and identified, respectively, as 'economic issues' by utilizing the same library databases detailed in section 8.6.1.3. However, unlike in the LCA, the input impact categories had to be manually characterised with the correct individual factors and CAS numbers, classified as 'economic issues', appropriately grouped, and assigned weighting.

Table 8.7. Inputs of each impact category in the LCCA with corresponding factors in USD (US Inflation Calculator, 2024). Raw materials via laboratory costs; Personnel costs (Indeed, 2024); CAPEX, OPEX, and NPV (Srinophakun & Suwajittanont, 2022)

Impact category (unit)	Input	Factor
Raw material cost (USD/kg)	Process water	0.5
	Sulfuric acid	0.244
	Sodium hydroxide	1.1
	Potato starch	0.8
	α-amylase	48.71
	Glucoamylase	40
Personnel cost (USD/year)	Employment hours: High-skilled female	34,650.09
	Employment hours: High-skilled male	34,650.09
OPEX (USD/year)	OPEX	3,087,044
CAPEX (USD)	CAPEX	1
NPV (USD/year)	Net Present Value (NPV)	9,072,253.26

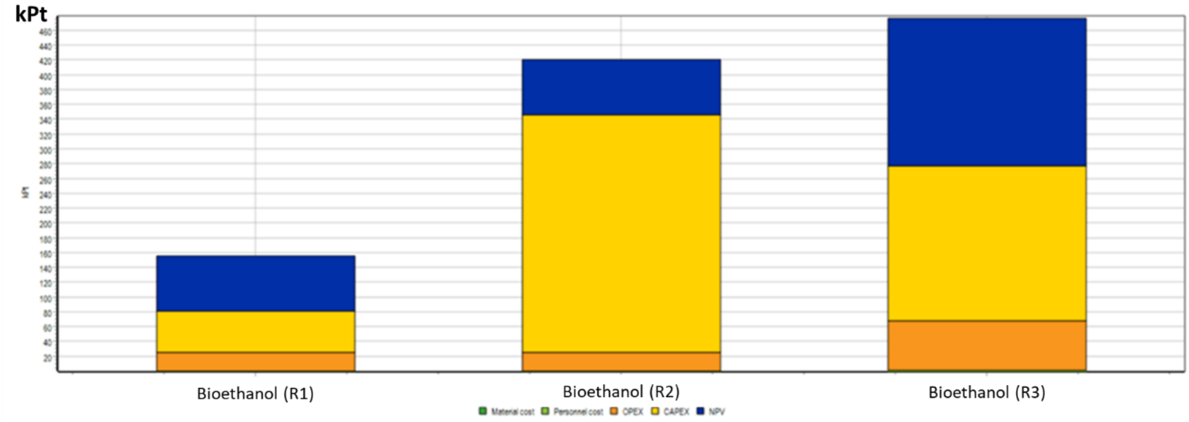

Figure 8.6. Single score (kPt) comparisons of bioethanol production pathways (R1-3) per economic impact category via LCCA: NPV (blue), CAPEX (yellow), OPEX (orange). Not visible on graph: Material cost (green) and Personnel cost (light green)

The factors were obtained via laboratory material costs per kg and Srinophakun & Suwajittanont (2022). Costs were adjusted to inflation, if applicable (US Inflation Calculator, 2024). Process contribution analysis was also able to provide information on the relative contribution of impact category, albeit not to the extent of LCA. Moreover, due to the base pilot-plant scale of the project, (techno-)economic data had to be scaled appropriately, based on cost estimates from bioethanol production literature (Srinophakun & Suwajittanont, 2022). Nevertheless, the LCCA allowed the decision-makers to determine the most significant sustainability factors to implement into the economic dimension of the final, optimised MCDM framework.

8.6.2.4 System boundaries

Although SimaPro can also employ LCCA, the methodology did have some notable differences. The LCCA had the same gate-to-gate system boundaries, as outlined in Figure 8.5. However, in contrast to LCA, LCCA required more manual set-up. Because normalisation is not commonly applied in LCCA (Pré, 2016), this project did not include it. Key sub-criteria were defined based on the relative significance of each economic impact category within the threshold(s) of the system boundaries, collaborative decision-maker discussions, and in accordance to the ISO 14044 standard. SimaPro was able to provide a visual representation and comparison of the magnitudes of each individual impact category for bioethanol R1-3. Three key sustainability factors were selected, based on only the three most significant economic impacts in relation to bioethanol production via the LCCA: NPV, CAPEX, and OPEX (Table 8.8).

Table 8.8. Economic sub-criteria of the final and most optimised MCDM framework, in which kPt=LCCA single scores (Srinophakun & Suwajittanont, 2022)

(*kPt)	NPV	CAPEX	OPEX
R1	74.6	55.7	25.4
R2	74.6	321	25.4
R3	199	209	67.7

8.6.3 Social-LCA

The literature review found that the social dimension of green sustainability is often neglected (Ren et al., 2015; Mattioda et al., 2020), despite being one of the three pillars that govern sustainability (Bartelmus, 2013; Popovic & Kraslawski, 2015; Geidoessfer et al., 2017). Therefore, in order for (green) sustainability to be approached holistically, social-LCA must be incorporated into decision-making methodologies beyond simply a safety perspective. Social-LCA should focus on the direct and indirect impacts of life-cycle components on people and society, from livelihoods to social acceptability on various spatial-temporal scales (Popovic & Kraslawski, 2015; Mattioda et al., 2020; Bouillass et al., 2021). Social-LCA has to be conducted with site-specific data requirements on a case-to-case basis, albeit some generalised boundaries can be established (Dreyer et al., 2006).

In recent years, the social dimension of sustainability has drawn greater attention from decision-makers of various disciplines, who have become increasingly aware of its importance in a holistic approach towards green sustainability (Ren et al., 2015; Mattioda et al., 2020). Therefore, although it is not essential to integrate social-LCA with the other PSEs (Popovic & Kraslawski, 2015), the project employed and integrated social-LCA with LCCA and LCA. This PSE framework provided a more focused and holistic selection of sustainability sub-criteria for the bioethanol case study. However, due to the lack of accessibility to a specific software package, social-LCA could not be implemented via SimaPro. Said software package would have included accessibility to the social hotspots database that contain up-to-date, case-specific data—governance, community infrastructure, labour rights, etc.—of supply chains for over 57 economic sectors and 140 countries/regions (Social Hotspots Database, 2025). Instead, Ren et al. (2015) was used to help establish an approximate social-LCA based on holistic sustainability, due to its relative similarity to the experimental validation case study: a systematic integration of PSE tools with AHP-VIKOR for (i.e. starch-based) bioethanol production.

8.6.3.1 Goals & Scope

The social-LCA had to identify, understand, and evaluate the potential social impacts resulting from the life-cycle activities of the bioethanol case study. Like the LCA and LCCA, decision-maker backgrounds were varied to provide a more well-rounded decision-making process. Social-LCA was employed to examine, assess, and define the social dimension of the case study. Only the three most significant sustainability factors were incorporated into the final, optimised MCDM framework as the social sub-criteria.

8.6.3.2 Functional unit(s)

The functional unit was the same across the three PSE tools: bioethanol, kg.

8.6.3.3 Inventory analysis

Ren et al. (2015) investigated three bioethanol production pathways via PSE tools, as opposed to solely potato starch in R1-3, with relatively similar starch-rich and crop-based feedstocks: cassava-based, corn-based, and wheat-based. Table 8.9 lists the social impact categories and corresponding (sub-)criteria that had been identified via semi-focused survey groups, stakeholders, and statistics (Ren et al., 2015). Each sub-criterion was given a subjective 'social performance' score from the combination of statistics, survey groups, and stakeholders; higher scores denoted better performances (Ren et al., 2015). The social dimension of the final, optimised MCDM framework was refined into three key sustainability factors, like in the AHP-VIKOR framework in Ren et al. (2015): social benefits (SB), socio-economic development (SED), and food security (FS) (Table 8.10).

Table 8.9. Social impact categories with corresponding sub-criteria and stakeholders/decision-makers in the social-LCA (Ren et al., 2015)

Impact category	Sub-criteria	Stakeholders/Decision-makers
Human rights	Equality & discrimination	Workers
	No forced labour	
	No child labour	
Working conditions	Fair pay	Workers
	Health & safety	
	Social benefits	
	Fair working hours	
	Freedom of collective bargaining + association	
Cultural heritage	Community engagement	Local community
	Healthy & safe living conditions	
	Land migration, acquisition, and delocalisation	
	Respect of local wisdom + customs	
	Respect of indigenous people rights	
	Material resource accessibility	
	Non-material resource accessibility	
Socio-economic repercussions	Local development	Society
	Socio-economic development	
	Food security	

	Horizontal conflict	
	Tech + knowledge transference	
Governance	Corruption-free	Value chain actors
	Public commitments to sustainability	
	Fair competition	

Table 8.10. Sub-criterion decision-maker scores of the social dimension of the final and most optimised MCDM framework, based on Ren et al. (2015)

Scores	SB	SED	FS
R1	8.75	8.75	9.75
R2	7.00	8.75	9.75
R3	0.25	1.25	9.75

8.6.3.4 System boundaries

According to Ren et al. (2015), the bioethanol system boundaries had consisted of the following: bioethanol production, agricultural crop production, crop transportation (~300 km from agricultural centre to plant), and bioethanol transportation from plant to market (~500 km). Key sub-criteria were defined based on the relative significance of each social impact category (Table 8.9) within relatively similar system boundaries to Figure 8.5 (i.e. gate-to-gate), decision-makers, and in accordance with a socially-adapted ISO 14044 standard.

8.7 Integration of PSE tools with MCDM

Sections 7.2 and 7.5 outlined the step-by-step MCDM methodologies that constituted the FAHP-VIKOR & PROMETHEE-II framework. The criteria and sub-criteria of this case study (Tables 8.6, 8.8, and 8.10) were applied to the aforementioned framework, with “fuzzy” logic in the first- and second-level pairwise comparison matrices (Appendices AD and AE, respectively), to calculate the “global” criteria weights (Table 8.11) and the following “local” sub-criteria weights: W_o, W_c, W_s, and W_i (Table 8.12). The global weights were subsequently utilised to derive sets of rankings for bioethanol production case study, using the sub-criteria established by the PSE tools. It should be noted, that the global weighting methodology could also prove to be useful by itself, for individuals to organisations at various spatial-temporal scales. Global weights could be utilised to illustrate the relative importance of each criteria and thus highlight potential weighting issues to be amended. However, what an organisation/individual(s) would do with this information, can depend greatly on various factors. For example, while a bank may discover (and expect) that their business model is (heavily) skewed towards the economic dimension, they may still be unwilling to enact significant change, if it proves to be too impactful on the economic dimension.

Table 8.11. "Global" criteria weights. These were required to calculate W_c and thus more reliable W_i values for pathway ranking (to 3 s.f.)

Criteria	Weights
A (env)	0.365
B (econ)	0.246
C (soc)	0.389

Table 8.12. "Local" sub-criteria weights of the bioethanol case study (to 3 s.f.)

	Non-c tox	Terrest tox	GW	NPV	CAPEX	OPEX	SB	SED	FS
W_c	0.0812	0.134	0.150	0.100	0.0727	0.0727	0.107	0.107	0.174
W_o	0.0694	0.115	0.112	0.0694	0.116	0.122	0.122	0.122	0.153
W_s	0.222	0.367	0.410	0.408	0.296	0.296	0.276	0.276	0.448
W_i	0.0758	0.126	0.131	0.0843	0.0926	0.0951	0.115	0.115	0.165

According to rankings listed in Table 8.13, R1 could be interpreted as the most overall optimal pathway for bioethanol production, as it was ranked highest by VIKOR and PROMETHEE-II based on W_i. Only W_i was processed for rankings, due to encompassing an overall balanced perspective in terms of weightings. That said, VIKOR had also offered R3 as a compromise solution; i.e., R3 was also viable as the most optimal pathway for decision-makers. This was more in-line with the FAHP rankings (R3=second highest), but in contrast to the last-place ranking via PROMETHEE-II. When compared to the ranking comparisons in section 7.5.1 for green NH_3 production, the bioethanol pathway rankings appear to be relatively similar in consistency across methodologies. However, the comparison is not entirely 1-to-1, perhaps partially due to the comparatively fewer pathways that were ranked in the bioethanol case study.

Table 8.13. Bioethanol production pathway rankings based on W_i. (*)Compromise solutions

Rankings (W_i)	FAHP	VIKOR	PROMETHEE-II
R1	3	1*	1
R2	1	3	2
R3	2	2*	3

Moreover, R1 as the overall most optimal pathway could be attributed to having the smallest production scale by volume of bioethanol distillate (Table 8.4), and thus overall lower impact magnitudes in (at least) the economic and environmental dimensions. Although outside of the project scope, the pilot-scale of the case study could have also been a potential factor that affected the rankings and created inconsistencies. In the original pilot-scale analysis via SimaPro (Figure 8.6), raw material cost was negligible, and the other economic costs—NPV, OPEX, CAPEX—had to be estimated from the larger-scaled production via feedstocks that were relatively similar in starch content to potatoes (Srinophakun & Suwajittanont, 2022). This was because R1-3 did not calculate for NPV, CAPEX, etc. at such a small scale, and no large-scale economic analysis studies were available that used potato starch as its (sole) feedstock. The adherence to the pilot-plant scale could be justified by what occurred upon upscaling R1-3 in the LCCA: increasingly higher raw material costs, with increasingly more questionable reliability.

Furthermore, the overall approach towards the social dimension may have had a potentially significant influence on the pathway rankings. The works of Ren et al. (2015) had to be used to help establish and employ the social-LCA without SimaPro, due to the lack of accessibility to the social hotspots database for up-to-date and case-specific data. Therefore, the social scores (Table 8.10) may not provide a completely accurate social-based representation of the project's experimental validation case study. That said, it can be argued that the social sub-criteria were sufficiently specialised and remains highly applicable to the project's bioethanol production case study. Thus, the selection of social sub-criteria can be deemed appropriate, particularly with regards to the project scope. The sub-criteria had also provided depth to the social dimension beyond (employee and workplace) safety, that provides a truly holistic approach towards green sustainability. However, to compare and improve upon the project findings, future research should still seek to implement social-LCA via SimaPro (or equivalent software platforms) and the social hotspots database. Nevertheless, with consideration to its scope and limitations, the project aims and objectives of chapter 8 (section 8.2) were fulfilled with relative satisfaction to what was achieved.

Section 8.8 covers the application of sensitivity analysis to evaluate the robustness of the final, optimised methodology framework.

8.8 Sensitivity analysis of the final, optimised methodology framework

W_i-based sensitivities of Q_i (FAHP-VIKOR) and *φ(a)* (PROMETHEE-II) have been plotted in Figures 8.7-.8, respectively, relative to incremental (+0.1) changes in weight for criterion A-C. R1 appears to be the most stable pathway via FAHP-VIKOR, with regards to the incremental changes in either of the three criteria. However, as proposed in section 8.7, this could be attributed to the much smaller production scale by distillate volume (Table 8.4); thereby, potentially rendering any notable sensitivity changes to be comparatively less notable. Comparatively, the Q_i results R2 and R3 are at their most stable in terms of environmental criterion, with no ranking changes from +0.1 to +0.9. In contrast, the rankings of R2 and R3 were subject to rank reversal in the social and economic criteria by +0.1 and +0.3, respectively. That said, VIKOR's overall stability can be deemed as significantly higher with the bioethanol case study than green NH_3 (Figure 7.3). This may be linked to the number of pathways and greater conflict(s) in criteria, which is known to cause and/or exacerbate rank reversal (Cinelli et al., 2014; Papathanasiou, 2021).

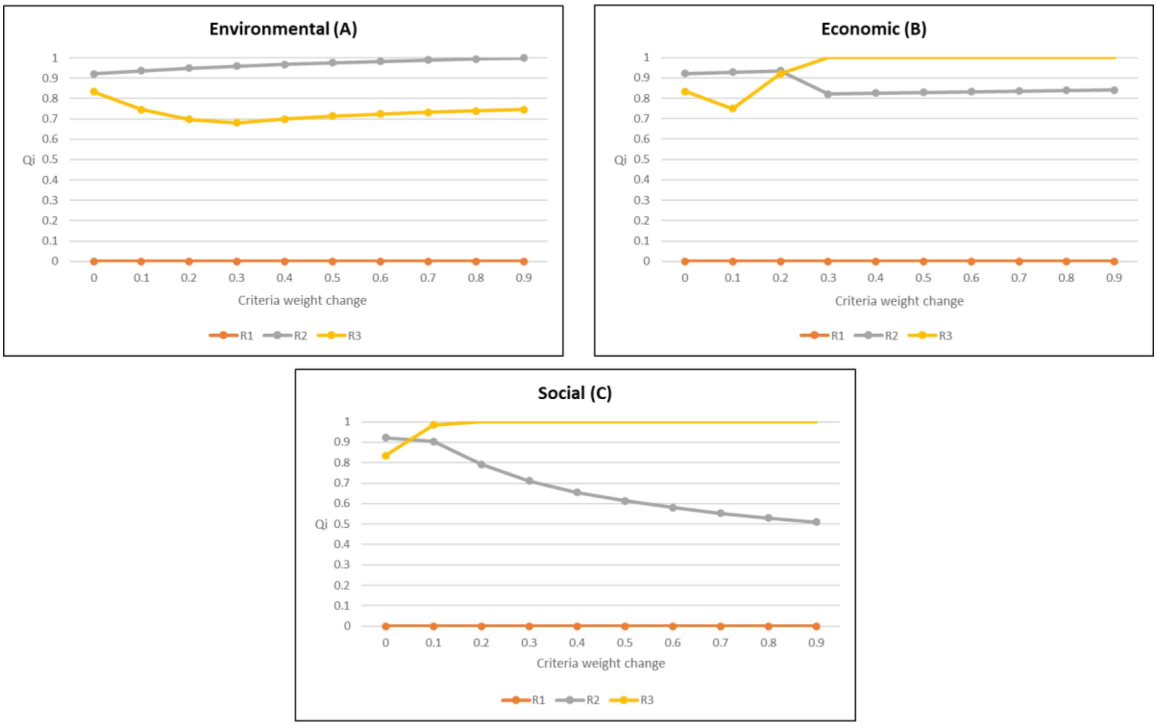

Figure 8.7. Q_i results relative to changes in environmental (A), economic (B), social (C) criterion weights for the bioethanol production pathways. When Q_i=1.0001, e.g. R3 in Economic and Social ≥+0.3, the line is barely within the graph

As was the case in section 7.6.3, *φ(a)* for bioethanol production has relatively high stability, with the same incremental (+0.1) changes to criteria weights, albeit to a comparatively far less extent than VIKOR in Figure 8.7. PROMETHEE-II is a highly stable and reliable ranking method, due to its use of a preference function (e.g. Gaussian), and net outranking flows being less sensitive to permutations (Gilliams et al., 2005; Wu & Abdul-Nour, 2020). Rankings were also consistent regardless of weight changes, except perhaps in the case of the environmental dimension. There is relatively minor ambiguity regarding the convergence of *φ(a)* values of R2 and R3 between +0.7 to +0.9 in criteria weight change. That said, most of the incremental weight changes, and the sensitivity analyses of the social and economic dimensions, had determined that R2 was ranked higher than R3.

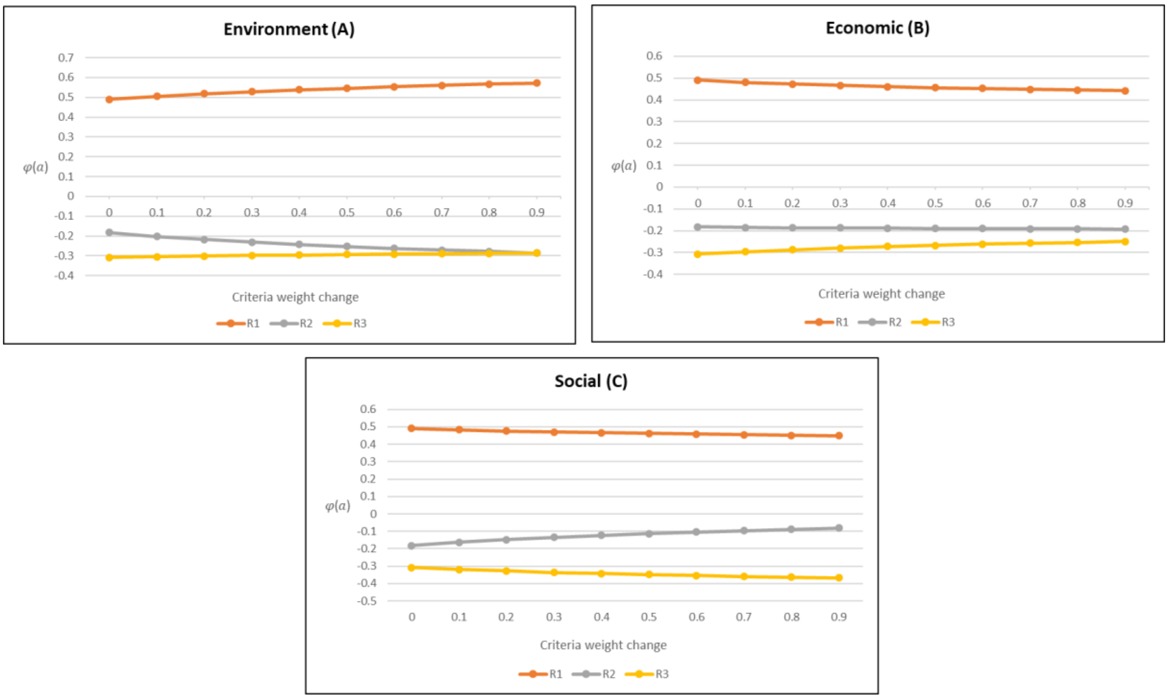

Figure 8.8. *φ(a)* results relative to changes in environmental (A), economic (B), and social (C) criterion weights for bioethanol pathways

8.9 Conclusions

Biofuels via renewable feedstocks have potential to become sustainable alternatives to conventional fossil-fuels (Qiao et al., 2022; Senthil et al., 2022; Guimarães et al., 2023; Ye et al., 2024). Biofuels, like bioethanol, can be green(er) fuel alternatives due to various multi-dimension benefits, such as reducing overall GHG emissions and addressing socio-economic development (Alam & Tanveer, 2020; Guimarães et al., 2023; Mansy et al., 2024). However, for biofuel production to be a viable long-term replacement to fossil fuels, it must address sustainability from a holistically green perspective. A pilot-scale case study of bioethanol production via potato starch feedstock was selected to validate the final, optimised methodology framework: the systematic integration of PSE tools (LCA, LCCA, and social-LCA) with FAHP-VIKOR & PROMETHEE-II. PSE tools were integrated to identify and derive the most relevant MCDM sub-criteria for this case study per criterion: environmental (Table 8.6), economic (Table 8.8), and social (Table 8.10).

In terms of W_i-based pathway rankings, R1 could be interpreted as the most overall optimal bioethanol pathway via VIKOR and PROMETHEE-II. R3 was also offered as a compromise solution via the former, in contrast to its last-place ranking via the latter. Overall, the bioethanol pathways appeared to be similar in terms of ranking consistency across methodologies. That said, the pathway rankings could have been affected by various factors, particularly the production scale (by distillate volume) of R1-3, and the reliance on literature to establish LCCA and social-LCA. Nevertheless, within the project's scope and limitations, the integration of PSE tools with FAHP-VIKOR & PROMETHEE-II was relatively successful.

In terms of sensitivity analysis, R1 seemed to be the most stable pathway via FAHP-VIKOR (Figure 8.7), while all three pathways were highly stable via PROMETHEE-II (Figure 8.8). Rank reversal was less common via sensitivity analysis, possibly due to the fewer number of pathways and conflicts among criteria/sub-criteria. Furthermore, the difference in stability with respect to changes in criteria weights for VIKOR versus PROMETHEE-II was notably less significant for bioethanol production than green NH_3 (Figure 7.4). Even so, VIKOR was arguably more stable with the bioethanol case study than green NH_3 (Figure 7.3). Future work should therefore seek to address the limitations and expand upon the scope(s) of the final, optimised methodology framework; specifically, the establishment of LCCA and social-LCA, production scale, and (potentially) the number of pathways. Moreover, specialised software platforms/packages, such as the social hotspots database (for social-LCA), should be implemented to establish (more) specialised LCCAs and social-LCAs with up-to-date, accurate, and case-specific data.

9. Discussion

The project sought to employ and/or enhance novel, holistically green and sustainable approaches within chemical process industries. In previous works (chapter 2), green sustainability and sustainable development have often been viewed solely via economic and/or environmental dimensions. Most notably, there is relatively little in-depth focus on green sustainability from a social(-political) perspective, despite their intrinsic significance in sustainability, such as the SDGs. Therefore, truly holistic approaches towards green sustainability are required. Moreover, the social dimension of green sustainability must be expanded upon to involve more than just overall safety (employee, workplace, etc.), before being integrated with other key sustainability criteria, wherever possible. At the very minimum, this should include social sub-criteria, such as policy applicability and public perception (Tables 7.6-.7), to achieve the ideal of holistically green sustainability and sustainable development.

Multi-criteria Decision Making (MCDM) could be the key towards incorporating holistically green sustainability in CPPs. Analytical Hierarchy Process (AHP) was by far the most common throughout the literature. But because individual methodologies have their weaknesses and limitations, it was highly recommended that individual methods were integrated to form hybridised MCDM frameworks, under a whole process design (WPD) philosophy. Additionally, process systems engineering (PSE) tools—life cycle assessment (LCA), social-LCA, and life cycle cost analysis (LCCA)—should be integrated with MCDM frameworks, to enable decision-makers to more reliably identify and select case-specific, key sustainability-related criteria and sub-criteria for MCDM.

In this thesis, four representative case studies were analysed and evaluated from a holistically green and/or sustainable perspective: sustainable water desalination, isopropanol (IPA) synthesis via isopropyl acetate, green ammonia (NH_3) production (chapters 4-6, respectively), and bioethanol production (chapter 8). The cases were selected, because they were relatively feasible, scalable, and cost-effective. That said, there was a reasonable degree of uncertainty with (and among) criteria and sub-criteria, particularly in regard to the social dimension, due to its comparative lack of depth in the literature. Consequently, it was difficult to ascertain the full extent of which each sustainability dimension (social, economic, etc.) can affect pathway rankings, as well as which pathways were the most optimal per dimension.

Nevertheless, each case study had served to validate the Posteriori MCDM frameworks of evolving complexity and increasingly better-defined impact categories (i.e., sub-criteria) regarding holistically green sustainability. Fuzzy AHP (FAHP) was utilised for sustainable water desalination, FAHP with Technique for Order of Preference by Similarity by Ideal Solution (FAHP-TOPSIS) for IPA, and FAHP-VIKOR with PROMETHEE-II for green NH_3 production. The final, most optimised methodology framework involved the systematic integration of FAHP-VIKOR & PROMETHEE-II with PSE tools (LCA, LCCA, and social-LCA) to derive the key sustainability factors of bioethanol production, instead of using a semi-random selection of sub-criteria based on literature and decision-maker perspectives. Unlike the first three (simulation-based) studies, bioethanol production was experimental-based and thus served to validate the final, optimised methodology framework under real-world conditions. Moreover, because it is often absent in the literature, sensitivity analysis was applied to evaluate overall robustness and stability of the MCDM frameworks.

For IPA, the most-to-least holistically optimal pathways were ranked as follows: Propylene Indirect Hydration (IAH) > Direct Propylene Hydration (PH) > Acetone Hydrogenation (AH). As for green NH_3 production, the overall rankings were as follows, albeit with some contention towards the middle rankings: hydropower electrolysis (HPEA) > wind turbine electrolysis (WGEA) > biomass gasification electrolysis/solar photovoltaic electrolysis (BGEA/PVEA) > nuclear high temperature electrolysis (NTEA). FAHP-TOPSIS and FAHP-VIKOR with PROMETHEE-II demonstrate that integrated (Posteriori) MCDM frameworks are highly adaptable, applicable, and relatively reliable in prioritising holistically green and/or sustainable pathways. The final, optimised methodology framework shows great promise as a novel approach towards implementing holistically green sustainability in CPPs. Specifically, the proposed methodology frameworks, regardless of complexity, have tremendous potential as a relatively intuitive decision-support tool for early-stage design and policy evaluation, that balances quantitative process modelling with qualitative sustainability assessments.

The systematic integration of PSE tools (section 8.7) for sub-criteria selection served to further refine the FAHP-VIKOR with PROMETHEE-II (FAHP-VIKOR & PROMETHEE-II) framework by deriving the key, case-specific sustainability factors based on the significance of their impact(s). However, the (potential) challenges and limitations should be noted and explored in further research; the use/reliance of secondary data from literature to establish approximate LCCA and social-LCA, the pilot-scale of the experimental validation case study, and its number of feasible bioethanol pathways. Potato starch has shown the potential to become a viable long-term renewable feedstock for bioethanol production (Taha et al., 2019; Suresh et al., 2020; Kumar et al., 2024), but further research must also consider the direct and indirect ramifications, beyond the scope of this project. For example, land usage impacts (costs, environmental, etc.) that would be intrinsically linked with the life cycle(s) of the starch-based bioethanol feedstock(s), as well as its potential for exacerbating food and water scarcity in certain regions (Ren et al., 2015; Suresh et al., 2020; Kumar et al., 2024).

Nevertheless, there is still significant (and growing) potential towards using the project's proposed methodology framework: a novel approach to incorporating and/or optimising holistically green sustainability in CPPs, regardless of the CPP system itself. At the bare minimum, "global" criteria weightings (Table 8.11) could be utilised for specific purposes in relation to an organisation, e.g. economic weighting(s) for banks, if/when "local" sub-criteria may be affected too much by uncertainties. That said, the project can easily be viewed as the beginning to this novel approach towards holistically green sustainability. Future research is highly recommended to explore further breakthroughs and potential advances; future work is expanded upon in section 9.1. To summarise, future research should address 1) the limitations and challenges of the final, optimised methodology framework; 2) how it should/could proceed beyond the current project scope and spatial-temporal scale(s).

9.1 Future works

Future works must consider the use of precise, accurate, and real-time data for key variables, such as individual and/or total cost estimations (section 6.5.2). Other key variables, such as operational costs, must also be explored during process simulation to further encompass a holistically green and sustainable WPD philosophy. Additionally, future works should seek to address the development and implications of policy on a case-to-case basis (section 5.4.2) via a systematic integration of established stakeholder engagement(s) with more personal, general populace perspectives; i.e., how people (dynamic stakeholders, hypothetical, or otherwise) respond and may/can influence case-specific policy, and vice versa. A more in-depth and case-specific exploration of socio-political variables should also be undertaken, to elevate and refine the proposed framework into a more comprehensive sustainability governance platform. This could be achievable via open and closed surveys, like Guati-Rojo et al. (2021) in section 6.6, but with a wider range and quantity of social/socio-political data that would be specialised for each individual case study. The main aim would be to avoid and/or minimise uncertainties, particularly from sources that were identified throughout the project. The aforementioned considerations should also serve to clarify and/or provide further experimental validation with future works.

Moreover, if possible, specialised software platforms and/or packages should be used in the application of (techno-)economic-based process simulation, social-LCAs, LCCA, and PROMETHEE-II for more accurate and reliable data analyses. Consequently, this would mitigate/remove the reliance on literature-derived values from secondary sources. Smart Picker Pro would be the ideal software platform for PROMETHEE-II, as Excel is acceptable but increasingly time-consuming on more ambitious scales. Furthermore, specialised software platforms can often require potentially lengthy training periods. Alternative software may prove to be acceptable, albeit this would depend on its the reliability and capabilities, as well as time and resources. SimaPro v9.6.0.1 is capable of implementing social-LCAs, but this capability is dependent on the additional purchase of the social hotspots database to produce up-to-date, accurate, and reliable results. However, this should not be a significant issue for future large(r)-scale projects. Therefore, excellent time management will be essential in future works, especially if upscaling is applied, whether in terms of plant capacity and/or number of CPP case studies.

Future works may also consider the implementation of Artificial Intelligence (AI), specifically via artificial neutral networks (ANNs). AI has already been implemented in sustainability(-related) fields and policies, such as the MIC2025 policy, for immediate and long-term strategic sustainability planning (Song et al., 2025). ANNs can be particularly suited for future, more complex cases, while also continuously improving with increasingly larger (potentially unstructured) data quantities (Misra and Li, 2020). That said, there are various challenges associated with ANNs; most notably, data quantity and high data computational power requirements (Misra and Li, 2020; Jeon et al., 2021). Furthermore, the data itself must be accurate and reliable, or ANNs would simply produce garbage-in/garbage-out scenarios (Wang et al., 2019; Misra and Li, 2020; Xiang et al., 2023). Therefore, if future works were to implement AI, the following factors must be considered at a minimum: sufficiently powerful hardware (e.g. graphical processing units, GPUs) that saves on time and money, and high data quantities of (sufficiently) high quality (Wang et al., 2019; Misra and Li, 2020; Jeon et al., 2021).

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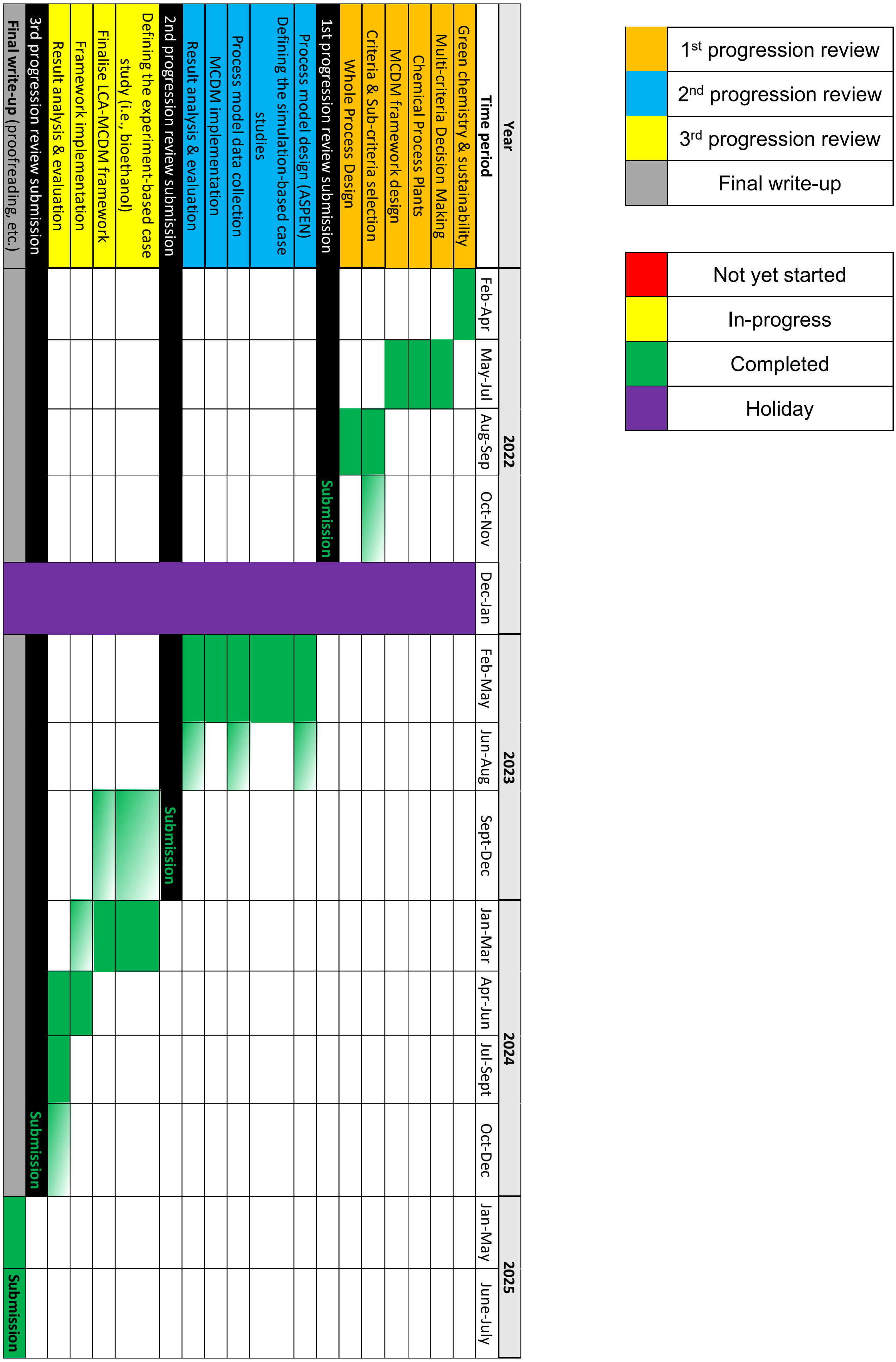
Appendices

Appendix A. Gantt chart of the PhD project (2022-25)



Appendix B. The 12 guidelines of GC, summarised from Anastas & Warner (1998)

Principle	Details
Prevention	Prevent waste from being generated in the first place, rather than finding ways to clean it up.
Atom economy	Ensuring that as much of the reagents are used as possible for the final product(s).
Less hazardous syntheses	Synthetic methods should not produce anything toxic to the environment and human health.
Design safer chemicals	Chemical toxicity should be reduced as much as possible, if not eliminated.
Safe(r) solvents & auxiliaries	Reduced usage, if not avoided wherever possible.
Energy efficiency	Energy usage should be minimised wherever possible.
Renewable material/feedstock usage	If feasible, renewable materials/feedstocks should be selected over non-renewable.
Catalysis	Catalytic reagents are preferred over stoichiometric reagents, wherever possible.
Reduced use of derivatives	Derivatisation process should be reduced, if not entirely avoided.
Design with product degradation in mind	At the end of their life cycle, products should break down into harmless products and not persist in the environment.
Real-time pollution prevention analysis	Real-time monitoring of analytical methodologies, so that potentially hazardous substances are not formed.
Prevent accidents	Substances (and their usage) should be selected with the intent to minimise accidents (e.g., fires and explosions).

Appendix C. Overall timeline of GC and sustainability

Year	Event(s)
1949 (Farias & Fávaro, 2011; De Marco et al., 2019)	Environmental concerns are first brought up at the 1949 United Nations Scientific

	Conference on the Conservation & Utilisation of Resources, in the USA
1962 (Farias & Fávaro, 2011; Barrow, 2012; Davis, 2012; De Marco et al., 2019)	“Silent Spring” by Rachel Carlson is published, ushering a new age of ecological and environmental awareness
1972 (Turner, 2008; Tobiszewski et al., 2009; Farias & Fávaro, 2011; De Marco et al., 2019)	“Limits of Growth” is published by Meadows et al., members of ‘The Club of Rome’, with various global subsystem model scenarios (1900-2100) Stockholm Conference further reinforces link between natural world and economy, with discussions on how to avoid societal collapse
1987 (Hopwood et al., 2005; Dahle, 2007; Bartelmus, 2013; De Marco et al., 2019)	Brundtland Report provides an overall accept definition of sustainability and sustainable development
1991 (Anastas & Warner, 1998; Woodhouse & Breyman, 2005; Tobiszewski et al., 2009; Farias & Fávaro, 2011; Sheldon, 2018; De Marco et al., 2019)	GC is introduced as a concept, as part of a US Environmental Protection Agency (EPA) programme, “Alternative Synthesis Routes for Pollution Prevention”
1997 (ACS, 2022)	Establishment of the Green Chemistry Institute (GCI) to promote sustainability in industry
1998 (Anastas & Warner, 1998)	The 12 guidelines of GC are established (Appendix B)
2000 (Galuszka et al., 2013)	Emergence of green analytical chemistry
2001 (De Marco et al., 2019)	GCI joins the American Chemical Society

Appendix D. Summary of literary findings for the discussed GC and sustainability-related topics: CEs (orange), and biomass (blue)

Title (short.)	Author(s)	Year	Case study/studies	Findings
CE – A New Sustainable Paradigm?	Geissdoerfer et al.	2017	English publications from Web of Science (WoS); 1950-2016 Differences between sustainability and CE in literature	CE = condition of sustainability CE + Sustainability = mostly researched in terms of env performance perspective; very little socially CE = emerging topic **BUT** simplified env perspective; long-term econ viability is often not discussed CE + Sustainability = no explicit definitions to differentiate

Conceptualizing CE: 114 definitions	Kirchherr et al.	2017	114 CE definitions (w/ 17 coding dimensions) via 155 journal articles + other bibliographic sources	CE literature = CE often equated to recycling; apparent neglect of reduce and recover; post-2012 implies shift from such framework Only ~1/3 literature refer to waste hierarchy; 40% via a waste systems perspective Authors view tenuous link to sustainable development; either econ or env, rarely social
Towards CE Implementation: Manufacturing Industry Comprehensive Review	Lieder & Rashid	2016	158 research papers from SCOPUS + WoS (1950-2015; English only)	Literature = multi-disciplinary w/ emphasis on econ benefits, resource scarcity, env impact, env science, industrial ecology End-of-life products =/= waste; but resources CE implementation has some success but large-scale requires radical changes; e.g., concurrent top-down + bottom-up
Catalytic Processes towards Biofuel Production: Palm Oil Biomass Biorefinery	Chew & Bhatia	2008	Pyrolysis of palm oil biomass in Malaysia → hydrogen + biofuels	Catalysis is important in hydrogen production Zeolite catalysts (e.g. ZSM-5 & Al-MCM-41) show promise due to porosity and acidity **BUT** thermal stability is a potential issue Heterogenous catalysts = need low-cost + faster, more efficient transesterification Catalytic cracking: MCM-41, SBA-15 = high selectivity Biorefineries: technologies need to

				know how to handle renewable feedstocks for biofuels **For other products, like long-chain HCs:** Fe + Co catalysts how promise with Fischer-Tropsch-Synthesis; Fe = sulphur tolerance, Co = faster reactions
MSW Pyrolysis w/ Iron-based Additives	Song et al.	2020	MSW pyrolysis + (iron oxide & iron ore as catalysts) in a series of fixed-bed reactor experiments Origin of the MSW = Datun Transfer station; Beijing	Iron-based additives → highly efficient pyrolysis; greater MSW weight loss Oxide > Ore, in terms of catalytic effect. Activation energy decreased to 151.76 vs 150.18 kJ/mol, respectively, from 180.32 kJ/mol Max pyrolysis conversion = 56.01% when 7.5% ore is added Increased production of CO_2, H_2, and CO Future studies should account for uncertainties; e.g. seasonality
MSW Pyrolysis Technologies: A review	Chen et al.	2015	A review on MSW pyrolysis; technologies, operation parameters, output products, environmental impacts	Most facilities are equipped w/ gas scrubbing, gasification/combustion tech Reactors = fluidised-bed, fixed-bed, rotary kiln, tubular **BUT** scale-up facilities only focus on tubular + rotary kiln Outputs = mainly heat/power; rarely syngas and/or biochar **BUT** the associated tech has greater flexibility Reactor type, pyrolysis temp, rate of heating, feedstock = significant

				impact(s) upon product composition/yield Liquid outputs should be avoided, due to chem composition complexity Potential contamination issues of gaseous outputs (e.g. HCl, SO_2, H_2S) + char; emission control devices are essential Product quality improvements → environmentally friendly pyrolysis

Appendix E. A full breakdown of the MCDM literature review by paper

Title (short.)	Author(s)	Year	Case study/studies	Method(s)	Criteria/Sub-criteria	Findings
MDCM/ Monte Carlo hybrid approach for sustainable solar site evaluation	Kannan et al.	2021	Solar site selection in the South Khorasan province, East Iran	Best-Worst Method (weighting) VIKOR + Grey Relational Analysis (prioritising solar site locations) Monte Carlo simulation (to compare prioritisation methods)	Soc = creating jobs, farmland distances, social acceptance Econ = construction cost, maintenance cost, initial investment Tech = substation distance, Env = ecosystem destruction, protected areas, catchment basin distances Risk = economic, investment, time delay	Birjand, the capital of the province, is the best location Most significant sub-criteria, in descending order: initial investment, construction cost, ecosystem destruction
Comparison among MCDA techniques: a novel method	Bandyopadhyay	2020	Amazon book sales at a local commercial library	TOPSIS MAUT MACBETH	Price; no. of book pages; book rating	Decision-Makers' subjective weightings: Rating = 0.39 Price = 0.33 Pages = 0.28

						Alt no. rankings (top 10, in descending order): TOPSIS = 9, 2, 1, 13, 19, 10, 4, 3, 6, 7 MAUT = 9, 1, 2, 4, 17, 20, 19, 5, 7, 14 MACBETH = 8, 17, 14, 20, 11, 4, 5, 18, 3, 7 Cumulative rating: MAUT > TOPSIS MACBETH is unacceptable, due to being the lowest value. Cumulative price: TOPSIS > MAUT, due to higher value Aggregate: TOPSIS = more dependable for ranking than MAUT
Best Manufacturing Procedure for Urea commercial production: AHP based TOPSIS	Ali et al.	2019	Urea production	AHP (relative criteria weights) TOPSIS (Alt closest to +ve ideal solution)	Profit, reliability, process flexibility, environment	AHP rankings: Hybrid system (.54), granulation (.24), prilling (.22) TOPSIS = prilling is most optimal (profit + reliability) → hybrid → granulation BUT granulation 1st for flexibility + environment Prilling is closest to -ve ideal for environment + flexibility
Motor vehicle chemical emissions based on preference ranking: PROMETHEE analysis	Beynon & Wells	2008	Raising the preference ranking of a vehicle (N=8), based on chemical exhaust emissions	PROMETHEE w/ the Gaussian function	CO_2, CO, HCO, NO_x (all in g/km)	Most preferred (w/ equal criteria weighting) = Toyota RAV4 Least preferred = Volkswagen Sharan Most important criteria = CO_2

						Least important criteria = CO
Evaluation of sites for the location of WEEE recycling plants in Spain	Queiruga et al.	2008	Selecting the most appropriate municipality, in Spain, for Waste Electrical & Electronic Equipment (WEEE) recycling plant installation	PROMETHEE w/ the Gaussian function	Objectives: Econ = Land costs, Personnel costs, Energy prices Infrastructure = Labour availability, inhabited area proximity, absence of other WEEE plants, Facility access, Proximity to metal/non-metal/hazardous substance facilities Legal = Env grants, local waste processing program availability	Region(s): Madrid (M), Andalucía (A) 1. Huelva (A) 2. Sevilla (A) 3. Algeciras (A) 4. Fuenlabrada (M) 5. Malaga (A) Reasons for being unsuitable, e.g. Castile & Leon = lack of sufficient infrastructure, low pop density Results are robust; decision-maker opinions will not significantly impact rankings, based on weightings + preference functions
Comparing MCDM Methods for Urban Sewer Network Plan Selection	Wu & Abdul-Nour	2020	Eight engineers (sanitary + civil) must decide the optimal construction plan to the reduce rainfall flow to a pumping station	AHP TOPSIS PROMETHEE-II (via Smart-Picker Pro decision software) ELECTRE-III (via ChemDecide) Delphi method (criteria identification)	Dynamic performance (+ve); Maintenance cost (-ve); Construction cost (-ve); Potential future profit (+ve); Env impact (-ve)	AHP weights: DP = 0.2349 Profit = 0. 2273 Construct = 0.2123 Main = 0.1814 Env impact = 0.1441 Final AHP scores: P2 = 0.363 P1 = 0.255 P3 = 0.2397 P4 = 0.1422 TOPSIS weights: Construct = 0.225 DP = 0.2188 Main = 0.2063 Profit = 0.1938 Env impact = 0.1563 TOPSIS averages (highest rank): Construct = P2 DP = P3 Main = P2

						Profit = P3 Env impact = P2 TOPSIS relative closeness: P1 = 0.6663 P2 = 0.5538 P3 = 0.4462 P4 = 0.2672 ELECTRE-III: P1 + P2 = 1st rank Differing 1st ranking among ascending/descending orders = inconclusive results PROMETHEE-II (alt ranking order, best to worst): 1, 2, 3, 4
Comparing MCDM Methods & Evaluating the QoL at Different Spatial Levels	Vakilipour et al.	2021	Objectively + holistically calculate quality of life, based on sub-districts of Districts 6 & 13, located in Tehran, Iran	VIKOR SAW TOPSIS ELECTRE	Socio-economic: 18, from 2011 census (Iranian Stats Centre) + relevant literature Environment: greenness, land surface temp, noise poll, air poll Accessibility to urban services + facilities: fire station, park, gas station, bus transit, urban bus, hospital, mosque, hospital + clinic, metro station	1st rank (District_Sub-district): TOPSIS = 13_09 VIKOR = 06_01 SAW = 13_09 ELECTRE = 13_09 Arithmetic mean rankings: D6 & D13 (N=24) 1st = 13_09 D6 (N=11) 1st = 06_03 D13 (N=13) 1st = 13_09 D6, 1st rank: TOPSIS = 06_09 VIKOR = 06_03 SAW = 06_01 ELECTRE = 06_03 D13, 1st rank: All methods = 13_09 Method stability (ranked highest to lowest): SAW TOPSIS ELECTRE VIKOR

PROMETHEE-II: Copper Exploration	Abedi et al.	2012	Exploration of porphyry copper deposits in Kerman, Iran (N=21, econ viable boreholes)	Fuzzy PROMETHEE-II w/ Gaussian + V-shaped w/ indifference Delphi method (weight extraction)	Geophysical: resistivity map, induce polarisation, metal factor, residual magnetic → reduced to pole magnetic → analytic signal of magnetic data Geochemical: molybdenum anomaly, copper anomaly, Additive map Geological: alteration zone, fault area, mineralisation indicators, host rock	Weightings: Highest = Additive map (0.1635); Lowest = Resistivity map (0.02295) Correction Classification Rate = 0.4286 Suitable boreholes (rating 4-5) = 1, 5, 6, 9, 10, 15
Multi-tier sustainable global supplier selection using a FAHP-VIKOR based approach	Awasthi et al.	2017	Sustainable global supplier selection (e.g. soc1), accounting for (1+n)th-tier sub-suppliers (e.g. env2)	FAHP-VIKOR FAHP: AIJ → aggregate criteria scores Fuzzy VIKOR: rank alts with respect to criteria Linguistic assessments → TFNs	**Stage 1** Econ: cost, flexibility, quality, dependability, innovativeness, speed Relationship quality: communication effectiveness, trust, electronic data interchange Env: water, materials, biodiversity, energy, emissions, waste + effluents, supplier env selection procedure Social: human rights, labour practices + decent work, product responsibility, society, supplier	S1 Criteria weights (eigenvector): Econ = 0.6 Env = 0.102 Soc = 0.066 RQ = 0.191 GR = 0.04 Local/Global greatest sub-criteria weights: Env1 = Materials (0.343/0.035) Soc1 = Labour + decent work (0.65/0.043) Econ1 = Cost (0.368/0.221) RQ1 = Trust (0.609/0.116) GR1 = Currency (0.633/0.026) S2 criteria weights (eigenvector): Env = 0.662 Soc = 0.337 Env2 = Materials (0.343/0.2272) Soc2 = Labour + decent work (0.65/0.2192) Supplier & Sub-supplier rankings,

					soc selection procedure Global risks: currency, political instability disruption, cultural compatibility, terrorism-related disruption **Stage 2** = repeat env + social	based on S_i, Q_i, R_i values: S3 > S1 > S2 SS3 > SS1 > SS2

Appendix F. Some of the most common risk/safety analysis techniques in the chemical processing industry

RA technique	Summary	Advantages	Disadvantages
Hazard & Operability Study (HAZOP) and its extended variant	Developed in 1963 by the Imperial Chemical Industries. An expert team conducts a systematic study (that includes "guidewords") to identify hazards and anything that could jeopardise CPP operability and/or productivity. Data is recorded onto a HAZOP worksheet **Extended:** include the use of dynamic simulation to identify any deviations in process parameters; rankings of risk consequences and their frequency; an	Provides a systematic and thorough evaluation of a system Potential to implement significant improvements to the evaluated system Deepens the understanding of chemical processes, as well as derive new knowledge	Potentially time-consuming and mentally-taxing (albeit depends on the system size and complexity) Often requires high level of expertise among experts for full effectiveness

	integrated risk matrix needs to be established; the results are ranked to prioritise the most important optimisation proposal(s)		
Layers of Protection Analysis (LOPA); (Willey, 2014)	Semi-quantitative evaluation of scenarios derived via previously applied hazard identification techniques, e.g. HAZOP. Includes a more thorough screening of risks and outcomes; also likelihood and severity via “order-of-magnitude”. If risk level is unacceptably high, implementation of additional protection layers is advised	Simplistic risk assessment tool, more thorough than HAZOP Identifies areas without safeguards of a sufficient quality, and helps decide layers of protection, if necessary Can also be applied for cost-benefit analysis Usable without software for risk simulation Useful in any process stage; design, emergency response, etc.	Often requires expert knowledge, skills, and experience to carry out Scenario-based; may not accurately assess individual risk Criteria for risk tolerance can vary among organisations

Human Reliability Analysis (HRA); (HSE, 2009)	Quantitative and qualitative to evaluate human factors associated with risk and performance. HRA approaches can be bespoke, depending on the industry.	Advantages vary based on approach; example: paired comparisons Effective judgements, even with scarce 'grey' data Experts can make individual comparisons, avoiding potential logistic issues Does not require calibration to make sound judgements on relative importance of human error/events	Disadvantages vary based on approach; example: paired comparisons Tasks may be too complex for straightforward comparison(s), further complicated by heterogenous tasks Comparisons may not be independent of each other Decision fatigue can become an issue over time

Appendix G. Notable ERGs and management system frameworks, established by the International Standards Organisation (ISO), in the chemical processing industry

ERG	Summary
ISO-20121	An international standard that offers advice and guidance for the best management of events, e.g. festivals; socially, economically, and/or environmentally. This relieves stress on (local) utilities and infrastructure

ISO-22301	The international standard for "business continuity management"; i.e. a business has the capability to continue delivering a pre-established quantity and quality of products/services within acceptable time frames, in spite of anticipated or unanticipated disruption (ISO, 2019)
ISO-28000	Aids organisations via an overarching security management system, in the assessment of security risks to their operational environment and supply chain(s)
ISO-9000 family	A certified quality management system for more than 1 million companies in >170 countries. Ensures that consumers are provided with "consistent, good-quality products and services" (ISO, 2022)
ISO-14000 family	A framework for effective environmental management, designed for any organisation type. Ensures everyone—from stakeholders to employees—that environmental impact(s) is/are considered and addressed (ISO, 2022)
ISO-45001	International regulation for occupational health & safety via safer, healthier work environment and "active" top management. Improves worker safety and lowers likelihood of injury. Also integrated with other ISO management standards, such as the ISO-9000 and ISO-14000 families (StandardsStores, 2022)
Seveso-III (Directive 2012/18/EU)	Aims to prevent major accidents involving hazardous substances in the EU, in addition to mitigating the impacts to the environment and human health. The direct

	focuses on establishments of relatively higher risk, e.g. nuclear plants (EC, 2022)

Appendix H-I. Model design parameters for water; TSS=Total Suspended Solids, SDI=Silt Density Index, TOC=Total Organic Compounds, DO=Dissolved Oxygen; NTU=Nephelometric Turbidity Unit (Feroz et al., 2012; Sana et al., 2005; Joy et al., 2021)

Parameter	Min	Max
Water temperature (°C)	21.3	26.9
Salinity (ppm)	34,000	34,400
pH	7.5	8.1
Turbidity (NTU)	1.5	1.65
TSS (mg/L)	-	1
SDI_{15} (mg/L)	0.45	-
TOC (mg/L)	5.12	5.38
Conductivity (mS)	52.34	56.22

Appendix H-II. Additional recommended design limits; GFD=Gallons/ft^2/day (Zaidi and Saleem, 2021)

Parameter		Recommended limit
SDI15 (mg/L)	**Max**	4
Turbidity (NTU)	**Typical**	0.1
	Conservative	7
System flux (GFD)	**Typical**	8
	Aggressive	10

Appendix H-III. Quality parameters for drinking (product) water (Petroleum Development Oman, 2012)

Parameter	Omani standard
TDS (mg/L)	<1000
Chloride (mg/L)	<600
Sodium (mg/L)	<400
pH	6.5-8.5
Turbidity (NTU)	1-5

Appendix H-IV. Model parameters for ion concentrations (Feroz et al., 2012; Sana et al., 2005; Joy et al., 2021

Ion	Concentration (ppm)
K^+	555
Na^+	10,730
Mg^{2+}	1450
Ca^{2+}	678
CO_3^{2-}	160

HCO_3^-	791
Cl^-	24,850
SO_4^{2-}	3060
Br^-	99

Appendix I-I. Optimised WAVE parameter data; 50 m^3/day (Bartram et al., 2023)

Permeate Flow (m^3/d)		Stages	Pressure Vessels	Elements	Membrane Type	Flux (GFD)	Price (USD/m^3)	Energy (kWh/m^3)
50		1	1	4	SW30XHR-400	8.3	1.325	6.72
		2	1	2	SW30XHR-400	8.3	1.327	6.72
		1	2	2	SW30XHR-400	8.3	1.295	6.53
		1	1	4	Seamaxx440	7.5	1.147	5.57
		1	2	2	Seamaxx440	7.5	1.032	4.78

Appendix I-II. Optimised WAVE parameter data; 200 m^3/day (Bartram et al., 2023)

Permeate Flow (m^3/d)		Stages	Pressure Vessels	Elements	Membrane Type	Flux (GFD)	Price (USD/m^3)	Energy (kWh/m^3)
200		1	3	6	SW30XHR-400	7.3	1.325	6.56
		2	2	4,5	SW30XHR-400	7.3	1.299	6.55
		1	6	3	SW30XHR-400	7.3	1.29	6.49
		1	2	8	SW30XHR-400	8.3	1.334	6.77
		2	3	3	SW30XHR-400	7	1.289	6.49
		2	2	2	SW30XHR-400	7.9	1.313	6.64
		2	1,2	5	SW30XHR-400	8.3	1.336	6.79
		2	2,3	3	Seamaxx440	8	1.156	5.63
		1	3	5	Seamaxx440	8	1.155	5.63
		1	5	3	Seamaxx440	8	1.155	5.63
		2	2	3,4	Seamaxx440	8.6	1.163	5.68
		1	4	4	Seamaxx440	7.5	1.147	5.57

Appendix I-III. Optimised WAVE parameter data; 500 m^3/day (Bartram et al., 2023)

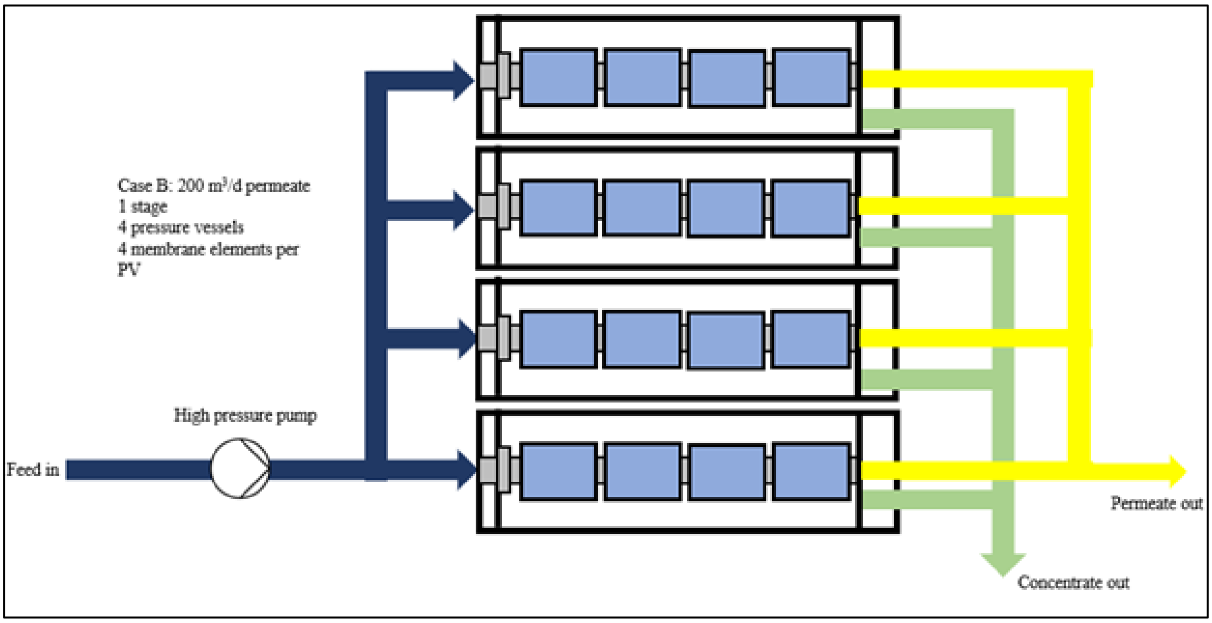
Permeate Flow (m^3/d)		Stages	Pressure Vessels	Elements	Membrane Type	Flux (GFD)	Price (USD/m^3)	Energy (kWh/m^3)
500		1	7	6	SW30XHR-400	7.9	1.319	6.68
		2	3/4.	6/6.	SW30XHR-400	7.9	1.32	6.68
		1	8	5	SW30XHR-400	8.3	1.335	6.78
		2	5	4	SW30XHR-400	8.3	1.333	6.77
		1	10	4	SW30XHR-400	8.3	1.325	6.72
		2	7	3	SW30XHR-400	8.3	1.319	6.68

		1	7	6	SW30XFR-400/34	7.9	1.281	6.43
		1	7	6	SW30XLE-440	7.1	1.229	6.1
		1	7	6	SW30-HRLE-400	7.9	1.278	6.41
		1	8	5	Seamaxx440	7.5	1.146	5.57
		2	4	5	Seamaxx440	7.5	1.141	5.53
		1	7	6	Seamaxx440	7.1	1.138	5.52

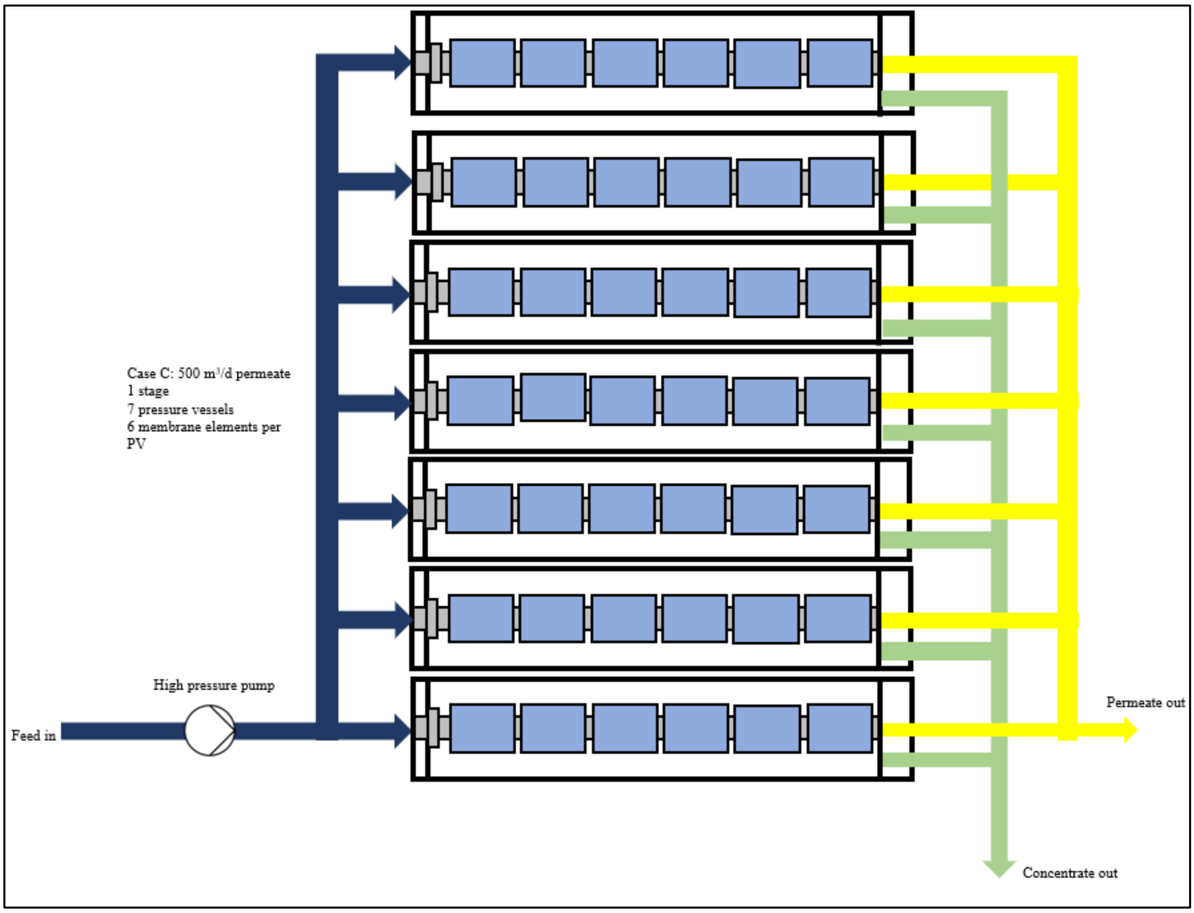
Appendix I-IV. Optimised WAVE parameter data; 1000 m^3/day (Bartram et al., 2023)

Permeate Flow (m^3/d)		Stages	Pressure Vessels	Elements	Membrane Type	Flux (GFD)	Price (USD/m^3)	Energy (kWh/m^3)
1000		3	6	4	Seamaxx440	8.3	1.155	5.63
		1	13	6	Seamaxx440	7.7	1.149	5.59
		1	13	6	SW30HRLE-440	7.7	1.277	6.41
		2	8	5	Seamaxx440	7.5	1.141	5.53

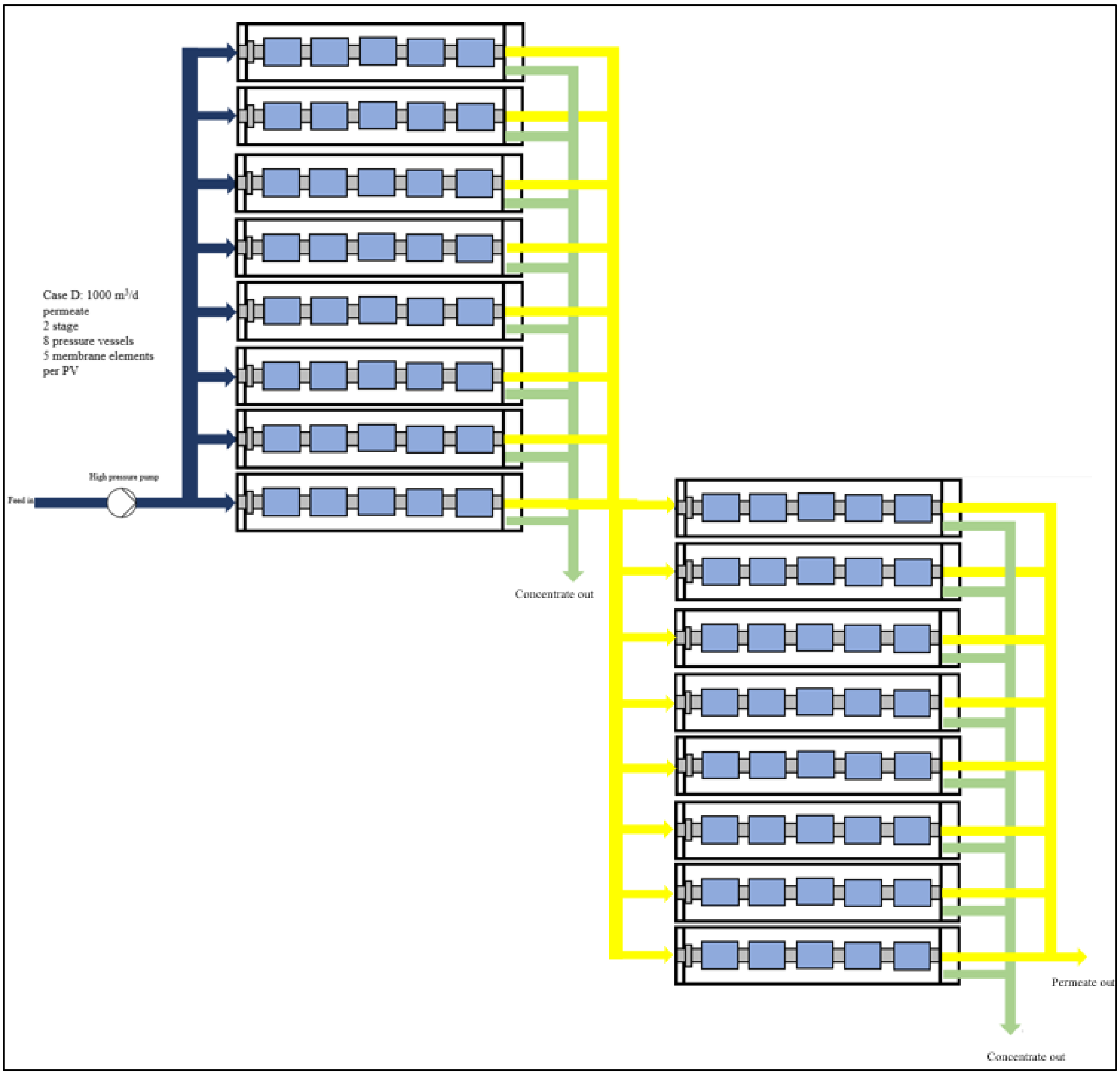
Appendix J-I. RO configuration for Case B (Bartram et al., 2023)



Appendix J-II. RO configuration for Case C (Bartram et al., 2023)



Appendix J-III. RO configuration for Case D (Bartram et al., 2023)



Appendix K-I. Calculated CAPEX costs (Kettani and Bandelier, 2020)

	Cost Parameter (USD/(m^3/d))	Case A Total Cost (USD $)	Case B Total Cost (USD $)	Case C Total Cost (USD $)	Case D Total Cost (USD $)
RO modules	70	3,500	14,000	35,000	70,000
Other equipment	450	22,500	90,000	225,000	450,000
Seawater intake/brine reject	100	5,000	20,000	50,000	100,000
Site preparation (construction)	400	20,000	80,000	200,000	400,000
Other costs (engineering, shipping, legal costs)	140	7,000	28,000	70,000	140,000
Total CAPEX (incl. 5% for contingency)	1,220	61,000	244,000	610,000	1,220,000

Appendix K-II. Calculated OPEX costs (without electricity) (Kettani and Bandelier, 2020)

	Cost Parameter (USD/m^3)
Membrane Replacement (20%/year)	0.3
Chemicals	0.08
Maintenance & Spare Parts (2% total CAPEX)	0.07
Brine Disposal and other externalities	0.04
Insurance (0.5% total CAPEX/y)	0.02
Labor	0.05
Total OPEX (incl 5% for contingency)	0.29

Appendix K-III. Specific electricity costs for each case per configuration (Bartram et al., 2023)

	Electricity Costs (USD/kWh)			
Configuration	Case A	Case B	Case C	Case D
100% Diesel	0.268	0.268	0.269	0.268
75% Diesel, 25% Solar	0.238	0.239	0.239	0.239
60% Diesel, 40% Solar	0.221	0.221	0.221	0.221

Appendix L. Code to calculate electricity costs; rq=required power, speccost=capacity/specific cost, pcgas=% gas generation (Bartram et al., 2023)

Electricity Costs

```
In[4]:= rq = 9.958; (*power required in kW*)
        (*Gas generation from diesel generators*)

In[36]:= pcgas = 0.75; (*percent required from gas generation*)
         gasgen = rq * pcgas; (*energy from gas gen required*)
         fuelp = 0.621; (*USD per L*)
         gasconsann = 0.4 * gasgen * 24 * 365
         (*0.4 L gas required per kWh*)
         (*(L/(kW h))*kW*24*365 h = L/year*)
         gaspriceann = gasconsann * fuelp (*$/year*)

Out[36]= 26170.

Out[37]= 1.625 × 10^4

In[38]:= (*Capital Costs*)
         capcost = 125 (*$/kW*) * gasgen

Out[38]= 933.6

In[39]:= (*Installation Costs*)
         installgas = 0.15 * capcost;

In[40]:= totalcapcostgas = capcost + installgas

Out[40]= 1074.

In[43]:= (*O&M*)
         OM = 0.02 (* USD/(kW h) *) * gasgen * 24 * 365 (*from Homer Energy*)

Out[43]= 1308.

In[44]:= annualopcost = OM + gaspriceann (*annual operating cost for diesel generator*)

Out[44]= 17560.

In[45]:= (*solar*)
         pcsolar = 1 - pcgas (*percent from solar*);
         peff = 0.183 (*efficiency of PV panel*);
         solpow = (pcsolar * rq) / peff (*solar power input, kW*)

Out[47]= 13.6

In[48]:= irrad = 5.58 (*solar radiation in kWh/d*);
         solarareaeq = solpow / irrad (*required area of PV array*)

Out[49]= 2.438
```

```
In[50]:= areaPV = (1762 / 1000) * (1037 / 1000.) (*m2*);
         numPVs = solarareq / areaPV (*number of photovoltaic cells*)
Out[51]= 1.334

In[52]:= panelprice = 700 (*USD*);
         capcostsol = numPVs * panelprice (*capital cost PV array*)
Out[53]= 934.

In[54]:= OMsol = 10 * solpow * 24 (*O&M, USD / (kW h/y) *);
         InvCap = 5 (*inverter capacity in kW*);
         numinv = solpow / InvCap
Out[56]= 2.721

In[57]:= InvPrice = 700 (*inverter price USD*);
         RepCost = 600 (*replacement cost*);
         Invcapcost = numinv * InvPrice;
         Invrepcost = numinv * RepCost;

In[61]:= installsolar = 1120 * pcsolar * rq
Out[61]= 2788.

In[62]:= totalcapcostsol = capcostsol + Invcapcost + installsolar (*total capital cost of solar-diesel hybrid*)
Out[62]= 5627.

In[63]:= totaloMcost = OM + OMsol (*total O&M costs*)
Out[63]= 4573.

In[64]:= totalOPEX = totaloMcost + gaspriceann (*total OPEX*)
Out[64]= 2.082 × 10^4

In[68]:= totalcapcost = totalcapcostgas + totalcapcostsol
Out[68]= 6700.

In[69]:= TotalNPC = totalcapcostgas + annualopcost * 20 + totalcapcostsol + OMsol * 20 + Invcapcost + Invrepcost
           (*Net Present Cost, USD*)
Out[69]= 4.267 × 10^5

In[70]:= speccost = (annualopcost + OMsol) / (50 * 365) (*specific operating cost*)
Out[70]= 1.141
```

Appendix M-I. Capital costs per energy configuration (Bartram et al., 2023)

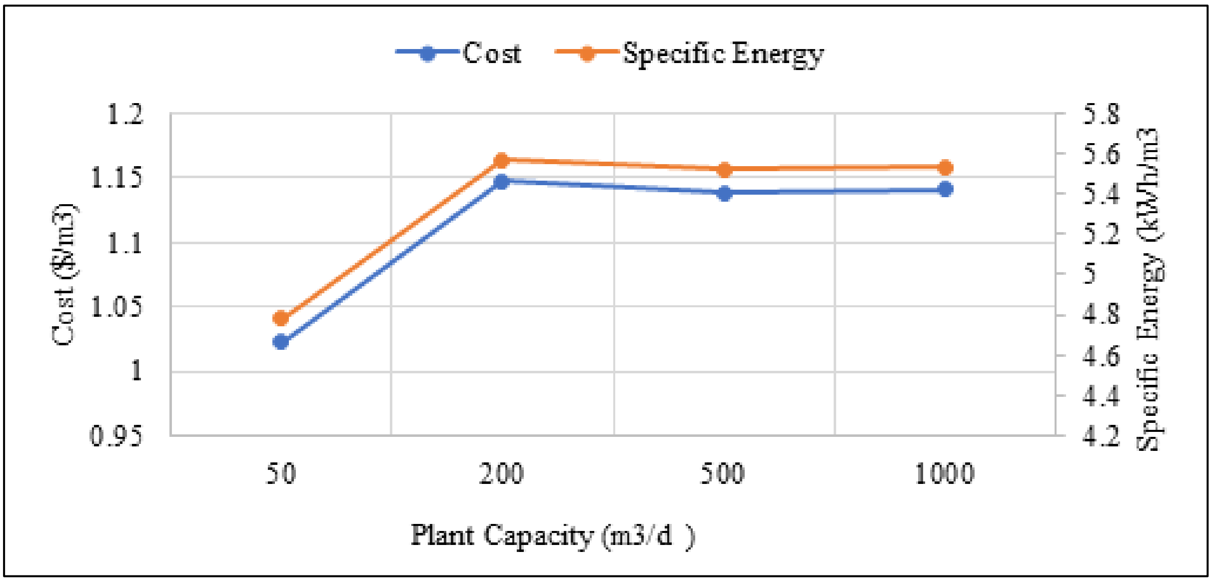
Case	Energy Configuration	Electricity Generation	Desal. Equipment	Total
A	100% Diesel	1,431	61,000	62,431
	75% Diesel, 25% Solar	6,700	61,000	67,700
	60% Diesel, 40% Solar	9,862	61,000	70,862
B	100% Diesel	6,673	244,000	250,673
	75% Diesel, 25% Solar	31,230	244,000	275,230
	60% Diesel, 40% Solar	45,970	244,000	289,970
C	100% Diesel	16,530	610,000	626,530

	75% Diesel, 25% Solar	77,380	610,000	687,380
	60% Diesel, 40% Solar	113,900	610,000	723,900
	100% Diesel	33,120	1,220,000	1,253,120
D	75% Diesel, 25% Solar	155,000	1,220,000	1,375,000
	60% Diesel, 40% Solar	228,200	1,220,000	1,448,200

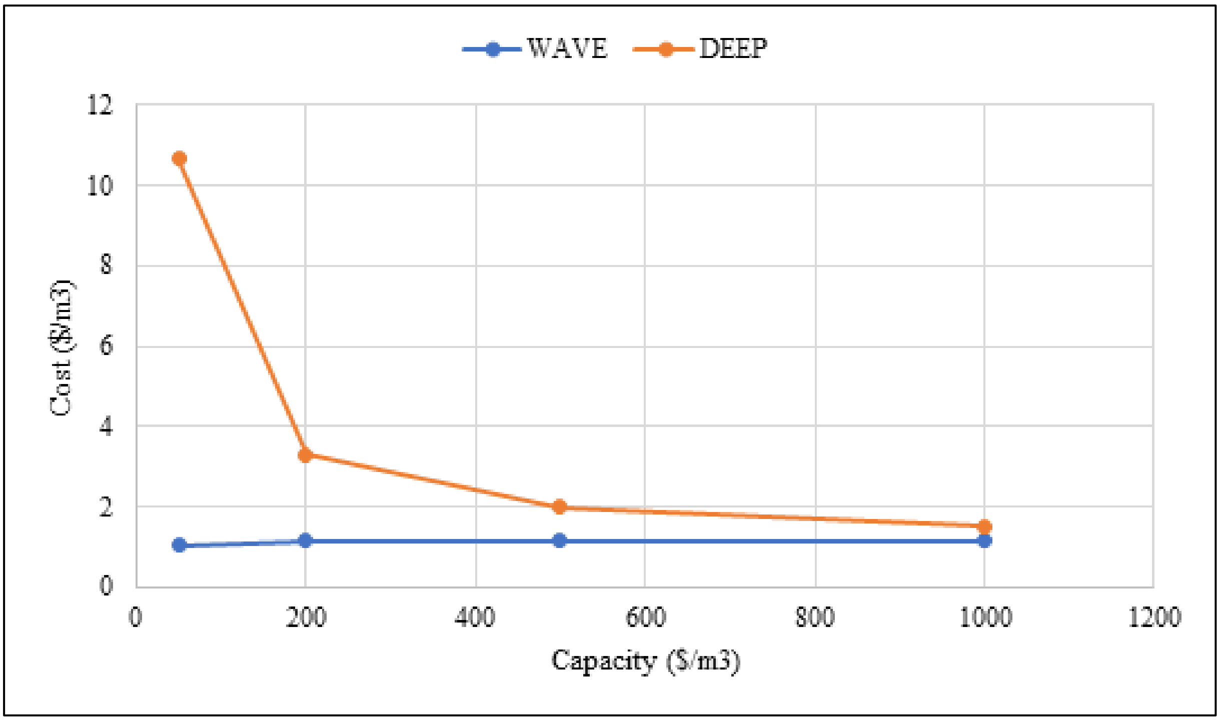
Appendix M-II. Specific energy costs per configuration

	Electricity Costs (USD/kWh)			
Configuration	Case A	Case B	Case C	Case D
100% Diesel	0.268	0.268	0.269	0.268
75% Diesel, 25% Solar	0.238	0.239	0.239	0.239
60% Diesel, 40% Solar	0.221	0.221	0.221	0.221

Appendix N-I. WAVE specific (energy and water) costs (Bartram et al., 2023)



Appendix N-II. DEEP specific costs (Bartram et al., 2023)



Appendix O. Breakdown of DEEP specific costs. SWC=Specific Water Cost, O&M=Operating & Maintenance (Bartram et al., 2023)

Parameter	Case A	Case B	Case C	Case D
Capacity (m^3/d)	50	200	500	1000
Initial SWC (USD/m^3)	10.67	3.27	1.99	1.50
Management Cost (USD/m^3)	8.04	2.01	0.80	0.40
Labor Cost (USD/m^3)	1.81	0.45	0.36	0.27
Total O&M Costs (USD/m^3)	10.03	2.95	1.65	1.16
Labor and Management Percent of Total SWC	**98%**	**83%**	**70%**	**58%**

Appendix P-I. Estimations for reactor equipment cost (Li et al., 2023)

Bit number	Device name	Housing material	Reaction tube material	Quality /t	Quantity	Unit price/10,000 RMB
R0101	Esterification reactor	S31603	S31603	151.6	2	1212.8

R0202	Hydrogenation reactor	Q345	Q345	208.6	2	417.2
Total					4	1630

Appendix P-II. Estimations for tower equipment cost (Li et al., 2023)

Bit number	Device name	Material	Quality /kg	Quantity	Unit price/10,000 RMB
T0101	Acetic acid recovery tower	S31603	83512.12	1	835.12
T0102	Propylene recovery tower	S31603	36521.63	1	146.09
T0301	Distillation column	Q345	72135.71	1	288.54
T0302	Ethanol and isopropyl alcohol one-effect tower	Q345	98523.94	1	394.10
T0303	Ethanol and isopropyl alcohol two-effect tower	Q345	132421.81	1	529.69
T0304	Ethanol extraction one-effect tower	Q345	40251.31	1	161.01
T0305	Ethanol extraction two-effect tower	Q345	21523.77	1	86.10
T0306	Extractant recovery tower	Q345	18254.18	1	73.02

T0307	Isopropyl alcohol purification tower	Q345	45124.51	1	180.50
Total				9	2694.15

Appendix P-III. Estimations for heater equipment cost (Li et al., 2023)

Name	Type	Material	Quality /kg	Quantity	Unit price/10,000 RMB
Circulation heating furnace	Cylindrical heating furnace	Q345R	10135.4	1	25.34
Circulation heating furnace		Q345R	20510.7	1	51.28
Total				2	76.62

Appendix P-IV. Estimations for heater exchanger cost (Li et al., 2023)

Bit number	Device name	Model	Material	Quantity	Unit price/ 10,000 RMB
E0101 B	Propylene heater	BES600- 1.651.606 -82.216- $\frac{4.5}{25}$ -2II	Q345R	2	5.93
E0102 B	Acetic acid heater	BES600- 1.651.606 -84.288- 4.525 -2 I	S31603	2	6.06
E0103	Acetic acid recovery tower precooler	BEM350- 0.6051.5994 -15.418- $\frac{3}{25}$ -2 I	S31603	2	1.92

E0104 B	Circulating propylene heater	BEM600-1.650.121-92.579-625-2II	Q345R S31603	2	6.56
E0105	Acetic acid recovery tower condenser	BEM1800-0.110.22−580.8-625−2II	S31603 Q345R	2	35.85
E0106	Acetic acid recovery tower reboiler	BEM600-1.1212.86−56.79-4.519-1I	S31603 Q345R	1	2.20
E0107	Propylene recovery tower condenser	BEM600-0.550.77−89.125−4.525-2II	Q345R	2	6.35
E0108	Propylene recovery tower reboiler	BEM600-0.7922.86−51.195−4.519−2 //	Q345R	2	4.07
E0201 B	Raw material heater	BES1400-5.45275.5-699.4-625-2 //	Q345R	2	42.96
E0202 B	Hydrogen heater	BES800-5.55.4527−199.39−625−2 //	Q345R	2	12.96
E0203 B	Circulating hydrogen heater-4	BEM600-5.55.454−114.96−4.519−2 //	Q345R	2	7.89
E0204 B	Circulating hydrogen heater-2	BEM600-5.55.46−89.394−4.525−2 //	Q345R	1	3.18
E0205 A	Reaction product cooler-1	BEM900-5.55.46-271.7-4.525−2 //	Q345R	1	8.65

E0206 B	Circulating hydrogen heater-1	BES1000-5.55.46−321.3-4.525−2 //	Q345R	1	10.14
E0207 A	Reaction product cooler-2	BEM600-0.1435.45-55.8-319-2 //	Q345R	1	2.17
E0208	Reaction product cooler-3	BES1200-5.4450.605−478.496-625−2 /	Q345R	2	29.71
E0209	Circulating hydrogen heater-3	BES1100-5.50.605−412.7-625-2 //	Q345R	1	12.88
E0301	Light tower precooler	BEM600-0.21670.605−48.3−325-2II	Q345R	2	3.90
E0302	Ethanol isopropyl alcohol one-effect tower	BEM400-0.13970.605−23.22-325-2II	Q345R	2	2.43
E0303	Precooler	BEM1500-0.110.275−729.5-625-2II	Q345R	1	22.39
E0304	Double effect distillation heat exchanger	BEM600-0.2750.605−44.9−4.525-2II	Q345R	2	3.69
E0305 B	Ethanol isopropyl alcohol two-effect tower	BEM400-0.2971.562−38.3−4.525−2II I	Q345R	1	1.65
E0306 B	Reboiler-1	BEM400-0.2970.121-28.4-319-2II	Q345R	1	1.35
E0307	Ethanol isopropyl alcohol two-effect tower	BEM1800-0.2971.76−709.5-619−2II	Q345R	1	21.79
E0308 B	Reboiler-2	BEM700-0.01651.562−159.4-4.525-2II	Q345R	1	5.28

E0309	Ethanol isopropyl alcohol two-effect tower	BES400-0.6051.5576−28.2−319-2II	Q345R	2	2.69
E0310	Reboiler-3	BEM400-1.540.0165-28.4-319-2 //	Q345R	2	2.70
E0311	Ethanol extraction two-effect tower	BEM500-0.01656.16−27.26-4.525-2II	Q345R	2	2.64
E0312	Reboiler-1	BES500-0.01320.605−35.986−325-2II	Q345R	2	3.15
E0313 A	Ethanol extraction two-effect tower	BEM450-0.111.562-27.2-319-2II	Q345R	2	2.63
E0314	precooler	BES400-0.6050.1177−21.099−325-2II	Q345R	2	2.27
E0315	Ethanol double effect extraction	BEM400-1.540.11−13.7−319−2II	Q345R	2	1.82
E0316	Heat Exchanger	BEM350-0.0550.605−23.435−319-2II	Q345R	2	2.40
E0217	Ethanol extraction two-effect tower	BEM1800-0.0440.22−580.8-625-2II	Q345R	2	31.53
E0318	reboiler	BEM500-1.5620.121−72.2−4.525-2II	Q345R	1	2.67
E0319	Extraction agent recovery tower precooler	BEM325-0.01430.605−15.2−319−2II	Q345R	2	1.91
E0320	Recovery extraction agent cooler-1	BEM600-0.110.22−37.9−4.525-2II	Q345R	2	3.27

E0321	Recovery extractant cooler-2	BEM700-0.1210.605−105.1-4.519-2 //	Q345R	1	3.65
E0322	Ethanol double-effect extraction heat exchanger-2	BEM1500-0.0770.22−404.9-625-2II	Q345R	2	25.29
Total					350.6

Appendix P-V. Estimations for gas-liquid separator prices, excluding installation & accessories fees (Li et al., 2023)

Number	Bit number	Model	Quantity	Quality /t	Price/10,000 RMB
1	V0102	Gas-liquid separator	1	0.251	6.28
2	V0202		1	3.232	80.80
3	V0301		1	0.186	4.65
4	V0302		1	1.056	26.40
5	V0303		1	4.119	102.98
Total/10,000 RMB				221.10	

Appendix P-VI. Estimations for storage tank cost (Li et al., 2023)

Name	Material	Volume / m^3	Quantity	Unit price /10,000 RMB
Propylene raw material storage tank	Q345R	4000	1	131.73
Acetic acid raw material storage tank	S31603	2000	2	458.24
Hydrogen raw material storage tank	Q345R	5000	1	107.40
Glycerin raw material storage tank	Q345R	16	1	7.13
Ethanol product storage tanks	Q345R	5000	1	336.09
Isopropyl alcohol product storage tank	Q345R	5000	2	336.09
Mixing tank	Q345R	1000	1	98.58
Mixing tank	Q345R	300	1	39.95
Total			10	1515.19

Appendix P-VII. Estimations for return tank cost (Li et al., 2023)

Name	Type	Material	Nominal volume	Quantity	Unit price/10,000 RMB

T0101 reflux tank	Horizontal oval head storage tank	Q345R	6	1	3.23
T0302 reflux tank			16	1	6.08
T0305 reflux tank			0.5	1	0.58
T0306 reflux tank			0.5	1	0.58
T0307 reflux tank			0.8	1	0.73
Total				5	11.18

Appendix P-VIII. Estimations for pump equipment cost (Li et al., 2023)

Bit number	Model	Operation mode	Power /kw	Quantity	Price /10,000 RMB
P0101	GDF40-20	Single pump	1.5	2	1.998
P0102	GDF80-50	Single pump	11	2	4.7
P0103	GDF100-19	Single pump	7.5	2	3.158
P0104	CQB32-60-160	Single pump	1.5	2	0.798
P0105	GDF100-32	Series connection	15	4	10.316
P0201	ISL100-80-125B	Single pump	5.5	2	0.2506
P0301	IH-65-40-250	Single pump	22	2	0.9606
P0302	IH65-50-160	Single pump	1.5	2	0.2506
P0303	ISL100-80-125B	Single pump	5.5	2	0.9606
P0304	CK32/13H	Single pump	2.2	2	0.2198
P0305	CQB32-60-160	Series connection	1.5	4	0.9812
P0306	IS125-100-250	Single pump	75	2	9.144
P0307	25MS--2.2	Single pump	2.2	2	0.66
P0308	40GDL6-12	Single pump	1.5	2	2.358
P0309	IX140-32-125A	Single pump	0.75	2	3.656
P0310	IX132-25-160A	Single pump	1.1	2	3.656
Total				36	44.1

Appendix P-IX. Estimations for compressor cost (Li et al., 2023)

Bit number	Model	Quantity	Price /10,000 RMB
C0101	Propylene feed compressor	1	20
C0201	Hydrogen feed compressor	1	40
C0202	Hydrogen cycle compressor	1	40
Total		3	100

Appendix P-X. Summary of total process equipment costs (Li et al., 2023)

Device name	Equipment cost/10,000 RMB
Reactor	1630.00
Tower equipment	2270.93
Heater	76.62
Heat Exchanger	350.61
Gas-liquid separator	221.10
Storage tank	1515.19
Reflux tank	11.18
Pump	44.07
Compressor	100.00
Total	6219.69

Appendix Q. Estimated assumptions of total project investment (Li et al., 2023)

I. Fixed Assets Engineering Expenses			
Project	**Rate**	**Price**	
		×10^4 RMB	**×10^4 USD**

1.Equipment prices			
Standard equipment	The price of the equipment is based on the manufacturer's inquiry, and the insufficient part is estimated by referring to the price of similar equipment	6219.69	956.8754
Non-standard equipment	Equipment weight × material price + processing fee = equipment price = 2.5 × material price × equipment weight		
2.Equipment internal filler purchase fee			
The internal filler purchase fee is calculated as 3% of the equipment fee.		186.59	28.70615
3.Piping and instrumentation automatic control system fees			
Project	**Rate**	**Price**	
		×10^4 RMB	**×10^4 USD**
Process piping fees	36%	2239.09	344.4754
Instrument control fee	14%	870.76	133.9631
Electrical Equipment fee	12%	746.36	114.8246
Production tool purchase fee	2‰（1.2~2.5‰ required）	12.44	1.913846
spare parts purchase fee	6‰（5~8‰ required）	37.32	5.741538
Equipment miscellaneous expenses (transportation fee, loading and unloading fee, warehouse storage fee, etc.)	7‰（6.5~7.5‰ required）	435.38	66.98154
4.Other equipment purchase fees			
Project	**The rate is calculated based on the main equipment fee**	**Price**	
		×10^4 RMB	**×10^4 USD**
Utilities equipment purchase fees	1.20%	74.64	11.48308
Vehicle purchase fee	1%	62.30%	0.095846
5.Engineering installation costs			
Project	**Install factor**	**Price**	
		×10^4 RMB	**×10^4 USD**
Reactor	0.2	326.00	50.15385
Tower equipment	0.4	908.37	139.7492
Heat Exchanger	0.3	105.18	16.18154
Storage tank	0.3	454.56	69.93231
Pump	0.1	4.41	0.678462
Compressor	0.2	20.00	3.076923
Process piping	0.3	807.74	124.2677
Instrument and automatic control system	0.2	209.41	32.21692
Maintenance fees	Equipment investment*81.2%	74.64	11.48308
Management fee	Total salary*40%	480	73.84615
II. Construction project costs			
1.Direct cost			

Project	Rate	Price	
		×10^4 RMB	×10^4 USD
Land construction (production workshop and building construction)	25	1554.92	239.2185
Site construction (site cleaning, greening, etc.)	15	932.95	143.5308
2.Extra charges			
Based on direct costs, it is calculated according to a certain indirect rate. The indirect rate for this study is 10%		248.79	38.27538
III. Intangible asset expenses			
Project	**Rate**	**Price**	
		×10^4 RMB	**×10^4 USD**
Land use fee	Land price 288RMB/m2 Installation area 80,000RMB/m2	2304	354.4615
Technology transfer fee	Withdraw 10% of the equipment fee	621.97	95.68769
IV. Preliminary expenses			
Project	**Rate**	**Price**	
		×10^4 RMB	**×10^4 USD**
Basic reserve fee	=(Fixed assets + intangible assets + deferred assets) *10% (9-12% required)	1980.16	304.64
Prepare for price increases	Fixed assets*5%	821.84	126.4369
V. Working capital			
Project	**Rate**	**Price**	
		×10^4 RMB	**×10^4 USD**
Liquidity amount	Construction investment*15% (12~20% required)	2465.52	379.3108

Appendix R. Estimated assumptions of public works consumption (Li et al., 2023)

Project	Origin	Consumption	Unit price	Total cost	
				×10^4 RMB	×10^4 USD
-25°C Frozen brine	Factory Utilities station	800,000 tons/year	150 RMB/ton	12000	1846.154
Circulating cooling water	Water station	12 million tons/year	1 RMB/ton	1200	184.6154
30°C Air	Air compression station	80570Nm³/year	0.1 RMB/Nm 3	0.81	0.124615
Low pressure steam	Factory Utilities station	200,000 tons/year	200 RMB/ton	4000	615.3846

Medium pressure steam	Main plant Utilities station	59,000 tons/year	240 RMB/ton	1416	217.8462
High pressure steam	Main plant Utilities station	9,960 tons/year	240 RMB/ton	239.04	36.77538
Conduction oil	Main plant Utilities station	55,900 tons/year	7540 RMB/ton	42148.6	6484.4
Electricity	Park power supply	91.84 million degrees/year	0.75 RMB/kWh	6888	1059.692
Instrument air	Air compression station	6500Nm³/year	0.12 RMB/Nm 3	0.78	0.12
Total				67893.2	10445.11

Appendix S. Estimated assumptions of employee insurance (Li et al., 2023)

Serial number	Insurance name	% of total wages	Total cost	
			×10^4 RMB	×10^4 USD
1	Pension insurance	20%	244	37.53846
2	Unemployment insurance benefits	2%	24.4	3.753846
3	Medical insurance premium	6%	73.2	11.26154
4	Maternity Insurance	0.70%	8.54	1.313846
5	Injury insurance	0.90%	10.98	1.689231
6	Housing fund	8%	97.6	15.01538
Total			458.72	70.57231

Appendix T. Estimated assumptions of depreciation expenses (Li et al., 2023)

Project	Original value (10,000 RMB)	Depreciation life (year)	Residual rate (%)	Depreciation rate (%)	Annual depreciation	
					×10^4 RMB	×10^4 USD
Production equipment	6219.69	10	4%	9.60%	597.09	91.86
Construction	1554.92	20	5%	4.75%	73.86	11.36308
Utensils, Tools, Furniture	12.44	5	5%	19%	2.36	0.363077
Electrical Equipment	746.36	5	5%	19%	141.81	21.81692
Vehicle	62.2	5	5%	19%	11.82	1.818462
Total					815.12	125.4031

Appendix U. Estimated assumptions of taxes (Li et al., 2023)

Serial number	Project	Tax rate (%)	Tax ×10^4 RMB	Tax ×10^4 USD
1	Product sales revenue		156800	24123.08
2	Output tax	17	22782.9	3505.063
3	Total product cost		142056	21854.7
4	Purchase of raw materials and energy costs		144458	22224.25
5	Input tax	17	19842.7	3052.722
6	VAT	17	2940.21	452.34
7	City maintenance and construction fees	7	205.81	31.66308
8	Education surtax	3	88.21	13.57077
9	Sales tax and surcharges		3234.23	497.5738
10	Corporate income tax	25	2877.55	442.7

Appendix V-I. Sensitivity analysis of operating costs (Li et al., 2023)

Changing factors	Range of change				
	-10%	-5%	0%	5%	10%
Operating costs (10,000 RMB)	126314.4	133331.86	140349.33	147366.8	154384.26
Financial net present value (10,000 RMB)	114127.65	62348.54	16153.81	-25163.66	-65184.84

Appendix V-II. Sensitivity analysis of total product output (Li et al., 2023)

Changing factors	Range of change				
	-10%	-5%	0%	5%	10%
Total output (tons)	72000	76000	80000	84000	88000
Financial net present value (10,000 RMB)	930.39	9065.41	16153.81	32469.94	43883.13

Appendix V-III. Sensitivity analysis of product price (Li et al., 2023)

Changing factors	Range of change

	-10%	-5%	0%	5%	10%
Sales price (RMB/ton)	11700	12350	13000	13650	14300
Financial net present value (10,000 RMB)	-13570.15	1078.24	16153.81	33730.43	53603.81

Appendix W-I. Site temperature (Li et al., 2023)

The annual average temperature (℃)	16.4
Extreme maximum temperature (℃)	41.2
Extreme minimum temperature (℃)	-10
Average monthly temperature of the hottest month (℃)	33.2
Average monthly temperature of the coldest month (℃)	1.8

Appendix W-II. Precipitation (Li et al., 2023)

Average annual precipitation (mm)	1480
Most average monthly precipitation (mm)	198
Minimum average monthly precipitation (mm)	54
Average annual rainfall days	158

Appendix W-III. Thunder & lightening and frost-free period (Li et al., 2023)

Number of lightning days per year	45
Frost-free period	230~240 Day

Appendix W-IV. Humidity and air pressure

Maximum relative humidity	97
Minimum relative humidity	65
Average annual relative humidity	82
Maximum air pressure	0.1018
Lowest air pressure	0.1010
Annual mean air pressure	0.1016

Appendix W-V. Wind direction (Li et al., 2023)

Normal wind direction	SE (Southeast)
Frequency of normal wind direction (%)	13.4
Secondary wind direction	NW (Northwest)
Secondary wind direction frequency (%)	11.0
Strong wind rate of level 6 or above (%)	8.8

Appendix W-VI. Wind speed (Li et al., 2023)

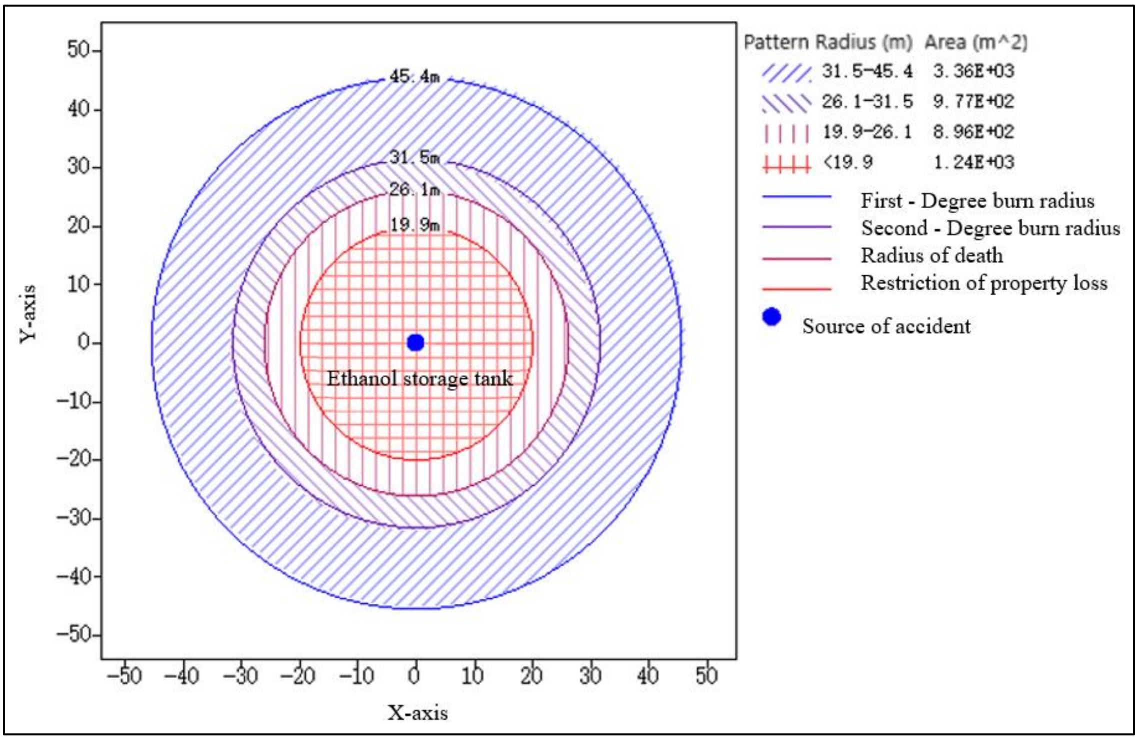
Average annual wind speed (m/s)	2.11
Maximum wind speed (m/s)	39.2
The annual average number of days with ≧level 6 gale throughout the year	40.6
The maximum number of days with ≧level 6 gale in the whole year	69

Appendix X-I. IPA injury range for the BLEVE pool fire model (Li et al., 2023)

Project	Forecast data (m)
Restriction of property loss	19.9
Radius of death	26.1
Second-degree burn radius	31.5

First-degree burn radius	45.5

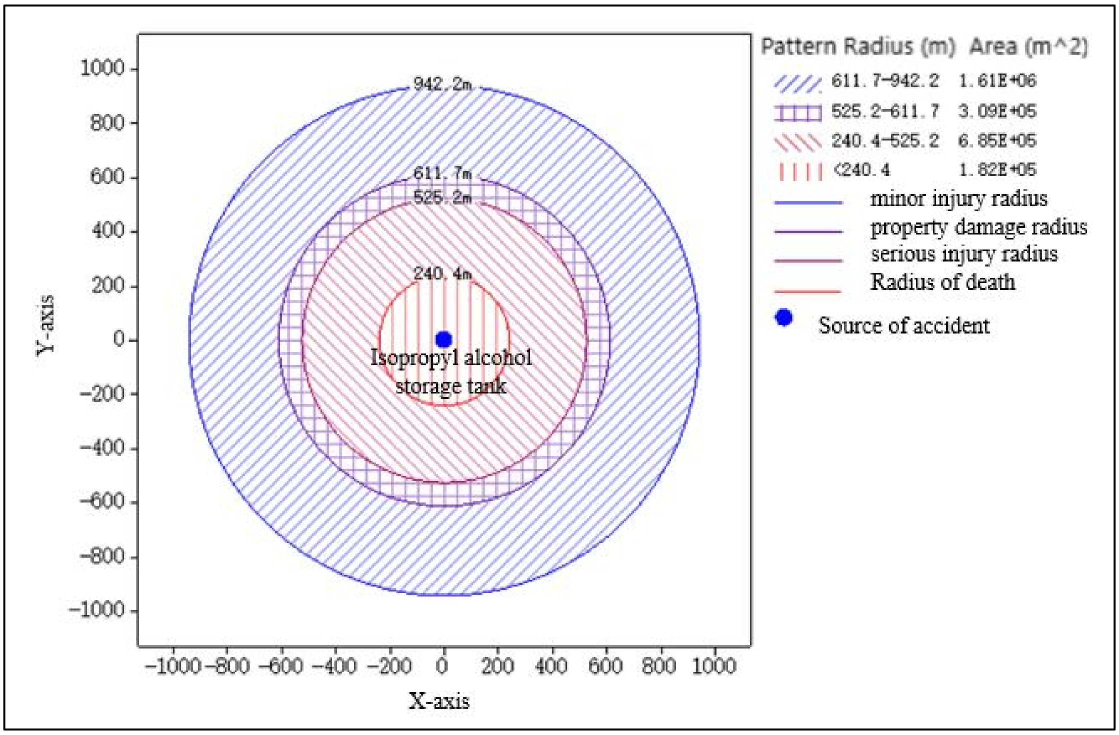
Appendix X-II. Pool fire simulation model (Li et al., 2023)



Appendix X-III. Vapour cloud explosion data (Li et al., 2023)

Project	Forecast data (m)
Radius of death	240.4
Restriction of property loss	611.7
Serious injury radius	525.2
Light injury radius	942.2

Appendix X-IV. Simulation model for vapour cloud explosion (Li et al., 2023)

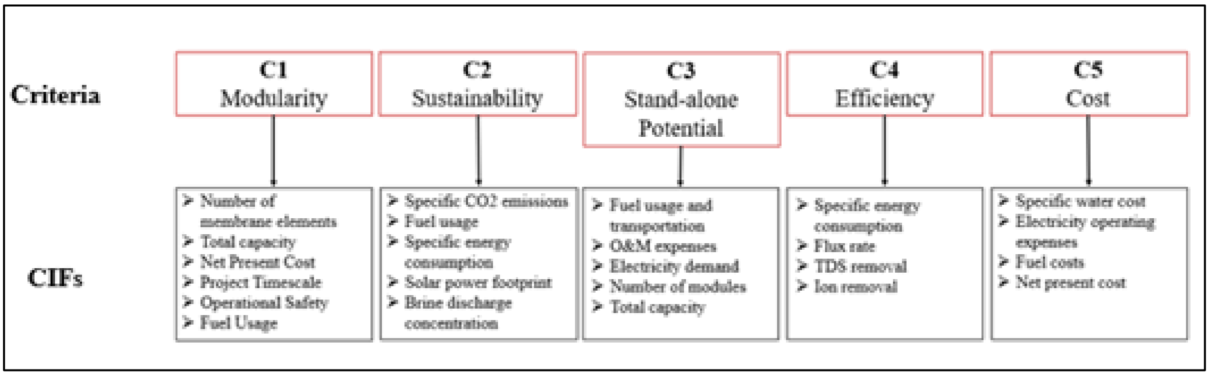


Appendix Y. Timeline of ammonia production (Pattabathula & Richardson, 2016)

Date	Event
1774	Gaseous ammonia is isolated for the first time
1785	Claude Louis Berthollet determines the chemical composition of ammonia
1898	Nikodem Caro and Adolph Frank discover that nitrogen could be "fixed" to form calcium cyanamide from calcium carbide, then hydrolysed (with water) to synthesise ammonia. However, significant energy requirements prevent large-scale production until the early-20th century
1906	Fritz Haber and Walther Nernst; the latter develops a process for ammonia production, in which a mixture of N_2 and H_2 is passed across an iron catalyst at 1000°C and 75 bar. But it is deemed unfeasible for large-scale production, due to no equipment being capable for it (at the time)

1910	Carl Bosch, Alvin Mittasch, and other BASF chemists develop a promoted iron-based catalyst, after testing >2,500 different catalysts
1913	Badische Anilin und Sodafabrik (BASF) constructs the first commercial H-B process ammonia plant (30 mton/day capacity) in Oppau, Germany
Mid-1960s	M.W. Kellogg revolutionises ammonia plant design by engineering a large, single-train ammonia plant, which is installed by American Oil Co., in Texas City, Texas (544 mton/day capacity)

Appendix Z. Sustainable water desalination sub-criteria



Appendix AA-I. C1 (Modularity) pairwise comparison matrix (Bartram et al., 2023)

	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	Weight
A1	1	0.5	0.333	2	0.5	0.5	3	2	2	4	2	0.5	**0.0865**
A2	2	1	0.5	2	2	2	2	2	0.5	3	2	2	**0.1160**
A3	3	2	1	3	0.5	0.5	3	2	2	4	2	2	**0.1299**
A4	0.5	0.5	0.333	1	0.5	0.333	2	2	0.5	3	2	2	**0.0679**
A5	2	0.5	2	2	1	0.333	0.333	2	2	3	2	2	**0.1047**
A6	2	0.5	2	3	3	1	3	2	2	3	2	2	**0.1396**
A7	0.333	0.5	0.333	0.5	3	0.333	1	0.333	0.333	2	2	0.5	**0.0578**
A8	0.5	0.5	0.5	0.5	0.5	0.5	3	1	0.5	2	2	2	**0.0650**
A9	0.5	2	0.5	2	0.5	0.5	3	2	1	2	3	2	**0.0977**
A10	0.25	0.333	0.25	0.333	0.333	0.333	0.5	0.5	0.5	1	0.5	0.333	**0.0281**

A11	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.333	2	1	0.5	**0.0413**
A12	2	0.5	0.5	0.5	0.5	0.5	2	0.5	0.5	3	2	1	**0.0652**
Sum	**14.583**	**9.333**	**8.75**	**17.333**	**12.833**	**7.333**	**23.333**	**16.833**	**12.167**	**32**	**22.5**	**16.833**	

Appendix AA-II. C2 (Sustainability) pairwise comparison matrix (Bartram et al., 2023)

	A1	**A2**	**A3**	**A4**	**A5**	**A6**	**A7**	**A8**	**A9**	**A10**	**A11**	**A12**	**Weight**
A1	1	0.333	0.25	3	2	2	3	2	2	4	3	3	0.1142
A2	3	1	0.5	2	3	2	4	3	2	4	2	0.5	0.1351
A3	4	2	1	4	3	3	4	3	2	4	3	3	0.1898
A4	0.333	0.5	0.25	1	0.333	0.25	3	0.5	0.333	3	2	0.5	0.0474
A5	0.5	0.333	0.333	3	1	0.5	3	2	2	4	2	2	0.0870
A6	0.5	0.5	0.333	4	2	1	3	3	2	4	2	2	0.1062
A7	0.333	0.25	0.25	0.333	0.333	0.333	1	0.333	0.25	3	2	2	0.0431
A8	0.5	0.333	0.333	2	0.5	0.333	3	1	0.5	3	2	2	0.0634
A9	0.5	0.5	0.5	3	0.5	0.5	4	2	1	3	2	2	0.0831
A10	0.25	0.25	0.25	0.333	0.25	0.25	0.333	0.333	0.333	1	0.333	0.25	0.0221
A11	0.333	0.5	0.333	0.5	0.5	0.5	0.5	0.5	0.5	3	1	0.5	0.0405
A12	0.333	2	0.333	2	0.5	0.5	0.5	0.5	0.5	4	2	1	0.0680
Sum	**11.583**	**8.5**	**4.67**	**25.167**	**13.917**	**11.167**	**29.33**	**18.167**	**13.417**	**40**	**23.333**	**18.75**	

Appendix AA-III. C3 (Standalone potential) pairwise comparison matrix (Bartram et al., 2023)

	A1	**A2**	**A3**	**A4**	**A5**	**A6**	**A7**	**A8**	**A9**	**A10**	**A11**	**A12**	**Weight**
A1	1	0.5	0.333	2	2	2	3	2	2	3	2	2	**0.1120**
A2	2	1	0.5	3	2	0.5	3	2	2	4	3	3	**0.1275**
A3	3	2	1	3	2	2	4	3	2	4	3	3	**0.1756**
A4	0.5	0.333	0.333	1	0.5	0.333	2	2	2	3	2	2	**0.0715**
A5	0.5	0.5	0.5	2	1	0.5	3	2	2	4	3	2	**0.0945**
A6	0.5	2	0.5	3	2	1	3	3	2	4	3	3	**0.1343**
A7	0.333	0.333	0.25	0.5	0.333	0.333	1	0.333	0.333	3	0.5	0.5	**0.0347**
A8	0.5	0.5	0.333	0.5	0.5	0.333	3	1	0.5	2	2	2	**0.0586**
A9	0.5	0.5	0.5	0.5	0.5	0.5	3	2	1	3	2	2	**0.0724**
A10	0.333	0.25	0.25	0.333	0.25	0.25	0.333	0.5	0.333	1	0.333	0.333	**0.0248**
A11	0.5	0.333	0.333	0.5	0.333	0.333	2	0.5	0.5	3	1	0.5	**0.0437**
A12	0.5	0.333	0.333	0.5	0.5	0.333	2	0.5	0.5	3	2	1	**0.0503**

Sum	**10.167**	**8.583**	**5.167**	**16.833**	**11.917**	**8.417**	**29.333**	**18.833**	**15.167**	**37**	**23.833**	**21.333**	

Appendix AA-IV. C4 (Efficiency) pairwise comparison matrix (Bartram et al., 2023)

	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	Weight
A1	1	1	1	3	3	3	2	2	2	2	2	2	0.1389
A2	1	1	1	3	3	3	2	2	2	2	2	2	0.1389
A3	1	1	1	3	3	3	2	2	2	2	2	2	0.1389
A4	0.333	0.333	0.333	1	1	1	0.5	0.5	0.5	0.5	0.5	0.5	0.0403
A5	0.333	0.333	0.333	1	1	1	0.5	0.5	0.5	0.5	0.5	0.5	0.0403
A6	0.333	0.333	0.333	1	1	1	0.5	0.5	0.5	0.5	0.5	0.5	0.0403
A7	0.5	0.5	0.5	2	2	2	1	1	1	2	2	2	0.0898
A8	0.5	0.5	0.5	2	2	2	1	1	1	2	2	2	0.0898
A9	0.5	0.5	0.5	2	2	2	1	1	1	2	2	2	0.0898
A10	0.5	0.5	0.5	2	2	2	0.5	0.5	0.5	1	1	1	0.0642
A11	0.5	0.5	0.5	2	2	2	0.5	0.5	0.5	1	1	1	0.0642
A12	0.5	0.5	0.5	2	2	2	0.5	0.5	0.5	1	1	1	0.0642
Sum	7	7	7	24	24	24	12	12	12	16.5	16.5	16.5	

Appendix AA-V. C5 (Cost) pairwise comparison matrix (Bartram et al., 2023)

	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	Weight
A1	1	0.333	0.333	3	2	1	2	3	1	3	2	0.5	0.0907
A2	3	1	2	3	2	2	3	2	2	3	2	2	0.1601
A3	3	0.5	1	4	3	2	3	3	2	4	3	2	0.1604
A4	0.333	0.333	0.25	1	0.5	0.333	1	0.5	0.25	0.5	0.333	0.333	0.0307
A5	0.5	0.5	0.333	2	1	0.5	2	1	0.5	2	1	0.5	0.0581
A6	1	0.5	0.5	3	2	1	3	2	0.5	2	2	0.5	0.0863
A7	0.5	0.333	0.333	1	0.5	0.333	1	0.5	0.333	1	0.333	0.25	0.0343
A8	0.333	0.5	0.333	2	1	0.5	2	1	0.5	2	1	0.5	0.0570
A9	1	0.5	0.5	4	2	2	3	2	1	3	2	1	0.1073
A10	0.333	0.333	0.25	2	0.5	0.5	1	0.5	0.333	1	0.5	0.333	0.0375
A11	0.5	0.5	0.333	3	1	0.5	3	1	0.5	2	1	0.5	0.0637
A12	2	0.5	0.5	3	2	2	4	2	1	3	2	1	0.1138
Sum	13.5	5.833	6.667	31	17.5	12.667	28	18.5	9.917	26.5	17.167	9.417	

Appendix AB. Sensitivity results for Ci+ relative to IPA criteria (A-D) weight changes

	Path	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
A (Tech)	PH	0.248009	0.254882	0.259727	0.263521	0.266659	0.269342	0.271691	0.273782	0.275667	0.277385
	AH	0.256727	0.26292	0.26717	0.27043	0.273079	0.275312	0.27724	0.278936	0.280448	0.281812
	IAH	0.495264	0.482198	0.473104	0.466049	0.460262	0.455346	0.451069	0.447282	0.443884	0.440803
B (Econ)		**0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**
	PH	0.248009	0.247977	0.247941	0.247903	0.247864	0.247824	0.247785	0.247745	0.247706	0.247667
	AH	0.256727	0.254784	0.253128	0.251682	0.250399	0.249244	0.248194	0.247232	0.246343	0.245518
	IAH	0.495264	0.49724	0.498932	0.500415	0.501738	0.502932	0.504021	0.505023	0.505951	0.506816
C (Env)		**0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**
	PH	0.248009	0.245923	0.244193	0.242707	0.241402	0.240236	0.23918	0.238215	0.237325	0.2365
	AH	0.256727	0.257975	0.258992	0.259852	0.260598	0.261257	0.261847	0.26238	0.262868	0.263315
	IAH	0.495264	0.496103	0.496816	0.497441	0.498	0.498507	0.498973	0.499405	0.499807	0.500185
D (Soc)		**0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**
	PH	0.248009	0.246411	0.245311	0.244485	0.24383	0.243291	0.242838	0.242449	0.242109	0.241809
	AH	0.256727	0.254338	0.252504	0.251007	0.249739	0.248637	0.247663	0.246789	0.245998	0.245275
	IAH	0.495264	0.499252	0.502184	0.504508	0.506432	0.508072	0.509499	0.510762	0.511893	0.512916

Appendix AC. Sensitivity results for Ci+ relative to green NH_3 criteria (A-D) weight changes

A (Env)	Path	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
	WGEA	0.2329	0.2335	0.2339	0.2343	0.2346	0.2349	0.2352	0.2354	0.2356	0.2358
	PVEA	0.1699	0.1645	0.1607	0.1577	0.1553	0.1531	0.1513	0.1496	0.1481	0.1467
	HPEA	0.3088	0.3122	0.3148	0.3168	0.3186	0.3202	0.3216	0.3228	0.3240	0.3250
	BGEA	0.1687	0.1742	0.1779	0.1807	0.1830	0.1849	0.1866	0.1880	0.1893	0.1904
	NTEA	0.1197	0.1156	0.1127	0.1104	0.1085	0.1069	0.1054	0.1042	0.1030	0.1020

B (Econ)		0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
	WGEA	0.2329	0.2334	0.2337	0.2340	0.2342	0.2344	0.2346	0.2348	0.2349	0.2351
	PVEA	0.1699	0.1721	0.1739	0.1755	0.1768	0.1780	0.1790	0.1800	0.1809	0.1817
	HPEA	0.3088	0.3048	0.3015	0.2988	0.2964	0.2943	0.2924	0.2907	0.2892	0.2878
	BGEA	0.1687	0.1690	0.1693	0.1696	0.1698	0.1699	0.1701	0.1702	0.1704	0.1705
	NTEA	0.1197	0.1207	0.1215	0.1222	0.1228	0.1233	0.1238	0.1242	0.1246	0.1250
C (Soc)		**0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**
	WGEA	0.2329	0.2346	0.2359	0.2371	0.2381	0.2390	0.2398	0.2406	0.2413	0.2419
	PVEA	0.1699	0.1719	0.1736	0.1750	0.1763	0.1774	0.1784	0.1794	0.1802	0.1811
	HPEA	0.3088	0.3086	0.3086	0.3085	0.3085	0.3085	0.3085	0.3085	0.3085	0.3085
	BGEA	0.1687	0.1671	0.1657	0.1646	0.1635	0.1626	0.1618	0.1610	0.1603	0.1596

	NTEA	0.1197	0.1178	0.1162	0.1148	0.1136	0.1125	0.1115	0.1106	0.1098	0.1090

D (Tech)		**0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**
	WGEA	0.2329	0.2293	0.2266	0.2245	0.2227	0.2212	0.2198	0.2186	0.2175	0.2166
	PVEA	0.1699	0.1662	0.1633	0.1610	0.1590	0.1573	0.1557	0.1544	0.1531	0.1520
	HPEA	0.3088	0.3149	0.3195	0.3233	0.3266	0.3294	0.3319	0.3342	0.3362	0.3381
	BGEA	0.1687	0.1663	0.1645	0.1630	0.1617	0.1605	0.1595	0.1586	0.1578	0.1570
	NTEA	0.1197	0.1234	0.1261	0.1283	0.1301	0.1316	0.1330	0.1343	0.1354	0.1364

Appendix AD. First-level linguistic comparison matrices of the bioethanol production case study. i) environmental; ii) economic; iii) social

i)	**Human non-c tox**	**Terr tox**	**GW**
Human non-c tox	E	RS	RF
Terr tox	S	E	RF
GW	F	F	E

ii)	**NPV**	**CAPEX**	**OPEX**
NPV	E	WI	F
CAPEX	RWI	E	E
OPEX	RF	E	E

iii)	**SB**	**SED**	**FS**
SB	E	RWI	RS
SED	WI	E	RF
FS	S	F	E

Appendix AE. Second-level (i.e. pathway-to-pathway within each sub-criteria) linguistic comparison matrices of the bioethanol production case study. Environmental=green; Economic=blue; Social=orange

Non-c tox	**CR=-0.0045**	**R1**	**R2**	**R3**	**W**
	R1	1	0.25	0.333	0.224869
	R2	4	1	3	0.462099
	R3	3	0.333	1	0.313032
Terr tox	**CR=-0.1777**	**R1**	**R2**	**R3**	**W**
	R1	1	0.25	0.333	0.218034
	R2	4	1	2	0.402572
	R3	3	0.500	1	0.379394
GW	**CR=0.0701**	**R1**	**R2**	**R3**	**W**
	R1	1	0.20	0.250	0.191426
	R2	5	1	3	0.428141
	R3	4	0.333	1	0.380433
NPV	**CR=0.016**	**R1**	**R2**	**R3**	**W**
	R1	1	1	0.25	0.244682
	R2	1	1	0.25	0.244682
	R3	4	4	1	0.510635
CAPEX	**CR=0.0577**	**R1**	**R2**	**R3**	**W**
	R1	1	0.2	0.25	0.174411
	R2	5	1	2	0.423951
	R3	4	0.5	1	0.401638
OPEX	**CR=0.0286**	**R1**	**R2**	**R3**	**W**
	R1	1	1	0.33	0.281087
	R2	1	1	0.33	0.281087
	R3	3	3	1	0.437825
SB	**CR=0.0909**	**R1**	**R2**	**R3**	**W**
	R1	1	2	5	0.433691

	R2	0.5	1	3	0.366768
	R3	0.2	0.333	1	0.199541
SED	**CR=0.0142**	**R1**	**R2**	**R3**	**W**
	R1	1	1	4	0.398452
	R2	1	1	4	0.398452
	R3	0.25	0.25	1	0.203096
FS	**CR=0.000**	**R1**	**R2**	**R3**	**W**
	R1	1	1	1	0.333333
	R2	1	1	1	0.333333
	R3	1	1	1	0.333333