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[Daniel Li](#)^{*}, [Mohamed Galal Hassan](#)^{*}, [Nuno Bimbo](#), [Zhaomin Li](#), [Ihab Shigidi](#)

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Article

Holistically Green and Sustainable Pathway Prioritisation for Chemical Process Plant Systems via a FAHP-TOPSIS Framework

Daniel Li ^{1,*}, Mohamed G. Hassan ², Nuno Bimbo ³, Zhaomin Li ⁴ and Ihab M.T.A. Shigidi ⁵

¹ Faculty of Engineering and Physical Sciences, University of Southampton, University Road, Southampton, SO17 1BJ, United Kingdom

² Faculty of Engineering and Physical Sciences, University of Southampton, University Road, Southampton, SO17 1BJ, United Kingdom; m.g.hassansayed@soton.ac.uk

³ Faculty of Engineering and Physical Sciences, University of Southampton, University Road, Southampton, SO17 1BJ, United Kingdom; n.bimbo@soton.ac.uk

⁴ Faculty of Engineering and Physical Sciences, University of Southampton, University Road, Southampton, SO17 1BJ, United Kingdom; zhaominli2023@163.com

⁵ Chemical Engineering Department, King Khalid University P.O. Box 39 Abha, 61411 etaha@kku.edu.sa

* Correspondence: ddl1r22@soton.ac.uk

Abstract: Multi-criteria Decision Making (MCDM) could be the key towards truly holistically green sustainability, within the context of chemical process plants (CPPs). ASPEN Plus v12.0 was utilised for two representative CPP cases: isopropanol (IPA) via isopropyl acetate, and green ammonia (NH₃) production. An integrated Fuzzy Analytic Hierarchy Process (FAHP) and Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) was modelled in MATLAB, to prioritise the holistically green and sustainable pathways. Life cycle assessments (LCAs) were employed to select the pathways, and the most suitable sub-criteria per four criteria: social, economic, environmental, and technical. In descending order of optimality, the pathways were ranked as follows for green NH₃ and IPA, respectively: Hydropower (HPEA) > Wind Turbine (WGEA) > Biomass Gasification (BGEA)/Solar Photovoltaic (PVEA) > Nuclear High Temperature (NTEA), and Propylene Indirect Hydration (IAH) > Direct Propylene Hydration (PH) > Acetone Hydrogenation (AH). Sensitivity analysis evaluated the FAHP-TOPSIS framework to be overall robust. However, there are potential uncertainties within and/or among sub-criteria, particularly in the social dimension, due to software and data limitations. Future research would seek to integrate FAHP with VIKOR, and Preference Ranking Organization Method for Enrichment Evaluation (PROMETHEE-II).

Keywords: multi-criteria decision making; AHP; TOPSIS; ammonia; isopropanol; life cycle assessment

1. Introduction

Multi-criteria Decision Making/Analysis (MCDM/A) is an instrumental research branch of decision-making theory [1]. 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) [1-3].

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) [2,3]. Due to their versatility and multi-dimensional applications, MCDM methods have been implemented throughout various disciplines, from

(municipal solid) waste management, to the production of raw materials [4-6]. MCDM/A can be utilised individually or as part of an integrated model, such as fuzzy Analytic Hierarchy Process (FAHP) or FAHP-Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS). Resultantly, different MCDM methods can provide varying ranking results based on their methodologies and the decision-makers themselves [7]. Decision-makers can then class and prioritise alternative solutions, based on criteria rankings, and choose which one is the overall “best” [8-11]. A simple example of a MCDM process is provided in Figure 1.

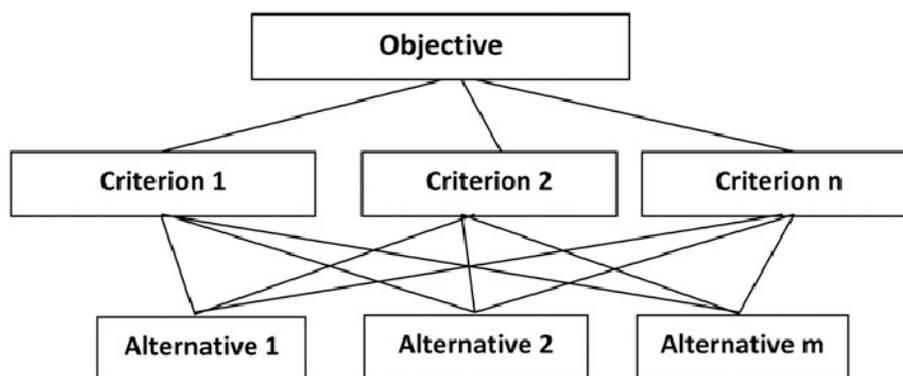


Figure 1. A simplified top-to-bottom MCDM process model [12].

In more recent years, MCDM/A methods have enabled decision-makers to approach green sustainability and sustainable development from a more holistic perspective. This is increasingly more important, as human society and the environment may suffer from severe and irreversible consequences [9-11,13]. 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 [14-17]. MCDM/A could be the key towards achieving green sustainability in chemical process plants (CPPs), in a holistic approach that has not been fully explored in past literature [18-22]. An integrated MCDM framework (FAHP-TOPSIS) was used to prioritise holistically green and/or sustainable pathways for two representative CPP case studies: isopropanol (IPA) synthesis via isopropyl acetate, and green NH_3 production.

2. Materials and Methods

2.1. FAHP-TOPSIS

The FAHP-TOPSIS model was coded in MATLAB by Li et al (2023). FAHP was used to derive the criteria weights for MCDM evaluation, based on said criteria and sub-criteria, with more accuracy and reliability than the standard AHP methodology. FAHP enabled the use of linguistic “fuzzy” variables for non-numerical (i.e. qualitative) data in MCDM, with Saaty’s relatively straightforward 1-9 pairwise comparison scoring system [20], so long as they were converted into corresponding and/or reciprocal triangular fuzzy numbers (TFNs). This was achieved via a linguistic-based fuzzy comparison matrix, as shown in Appendix A, in which linguistic-based judgements share corresponding TFNs [45] that can then be processed for straightforward application(s) in TOPSIS/additional MCDM ranking methods. TOPSIS was selected for reliable and accurate ranking, due to the availability of MATLAB code, and its many similarities to VIKOR. Section 3.3.1 outlines the TOPSIS methodology in a step-by-step process [23,29].

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 [18,20,22]. However, a certain level of complexity is still required to establish the context of the problem [22], albeit it also cannot compromise the flexibility of the AHP framework [12,21]. Due to its high flexibility, an increasing number of studies

have adopted hybridised AHP frameworks with fuzzy logic [6,23]. 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 [6,18,24]. 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 [23,25].

In comparison, TOPSIS was first developed and presented by Hwang & Yoon in 1981 [5,23,26,27]. 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) [5,23,25]. 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 [23,25,28]. TOPSIS also utilises criteria information to its fullest, while not requiring criteria to be independent, albeit this is only possible when all information is available and accurate [25,28]. Moreover, while there are advantages, TOPSIS does have two notable weaknesses: the requirement of vector normalisation for multi-dimensional problems [23,28], and the relative importance of the distances for the ideal solutions is not properly considered [25,27]. Additionally, a potential weakness/limitation to TOPSIS, is the use of crisp data values. Real-life scenarios are often fraught with uncertainty and relativity [26], which is why the incorporation of fuzzy logic to TOPSIS has become more popular [28,29].

A consistency level of $\leq 10\%$ ($CR \leq 0.1$) was deemed as acceptable [30,31]. To minimise the potential information loss during weight aggregation, the combined coefficient $u=0.5$ had been assigned. 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 [20,31,32], and thus depends on the surrounding circumstances. Fuzzy pairwise judgement matrices were established for the first layer index (Appendix B) and sub-criteria of each criterion (Appendices C-D). Said matrices were derived from group evaluations and literature findings. Because $CR \leq 0.1$ for all matrices, the consistency levels were deemed acceptable. To derive the objective weights, data must first be normalised in TOPSIS via vector normalisation, due to the differences in scales and/or units of measurement. Positive indicators and negative indicators were calculated via Equation 10 and Equation 11, respectively. Entropy weighting is utilised to calculate the objective (sub-criteria) weights, W_o . Section 3.3.2 elaborates on the calculations of objective (W_o), comprehensive (subjective) (W_c), and combination weights (W_i) in Eqs.12-17.

2.2. Case Studies

An IPA plant at the Sinopec Zhenhai Refining & Chemical Co., Ltd was simulated via ASPEN. 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 $\sim 99.99\%$, 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 [33,34]. 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 2 illustrates the process flow diagram, with the entire process simulation in Figure 3, and the plant layout in Figure 4.

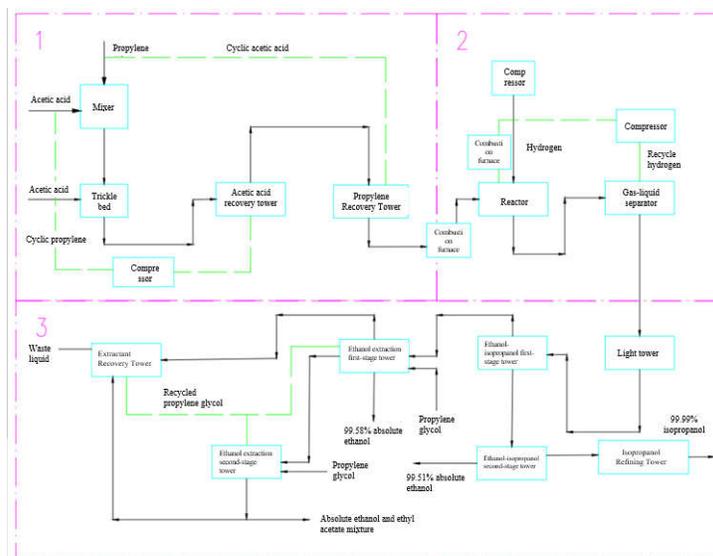


Figure 2. Process flow diagram for IPA synthesis; a=1) isopropyl acetate synthesis, b=2) isopropanol synthesis, c=3) isopropanol & alcohol refining.

A small-scale and modular green NH_3 production case study was simulated via Peng-Robinson (PENG-ROB) in ASPEN Plus v12.0. PENG-ROB is the one of the most popular property methods for NH_3 production, primarily due to its high reliability and applicability to various system types. This includes (relatively) non-ideal systems, in contrast to the Soave-Redlich-Kwong equation [35]. The standard 3:1 ratio between H_2 and N_2 was decided for the reaction, R-1, to synthesise liquid ammonia. The flowsheet model for clean, modularised NH_3 production (Figure 5) via hydrolysis can be divided into three 'modules', all developed by Arrarte (2022): gaseous hydrogen generation via the desalination of seawater coupled with PEM electrolysis (blue), gaseous nitrogen via ASU that utilises a cryogenic distillation process (red), and NH_3 synthesis (green).

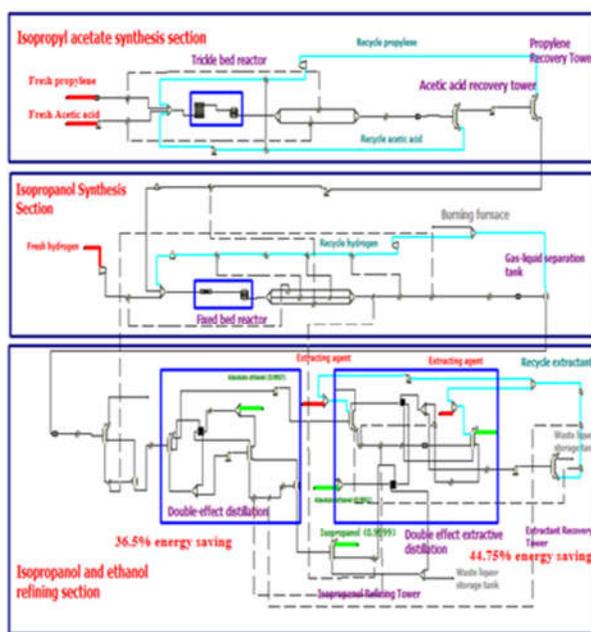


Figure 3. Complete process simulation per section, as modelled in ASPEN v12.

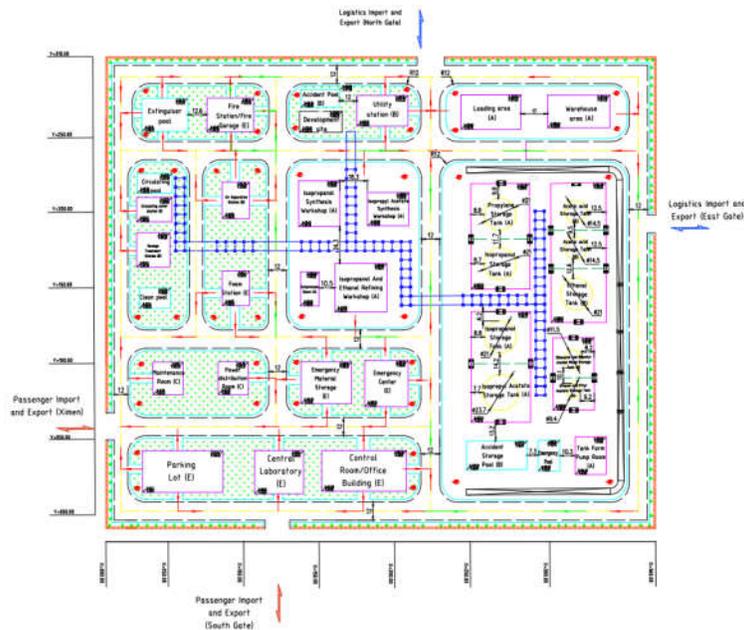
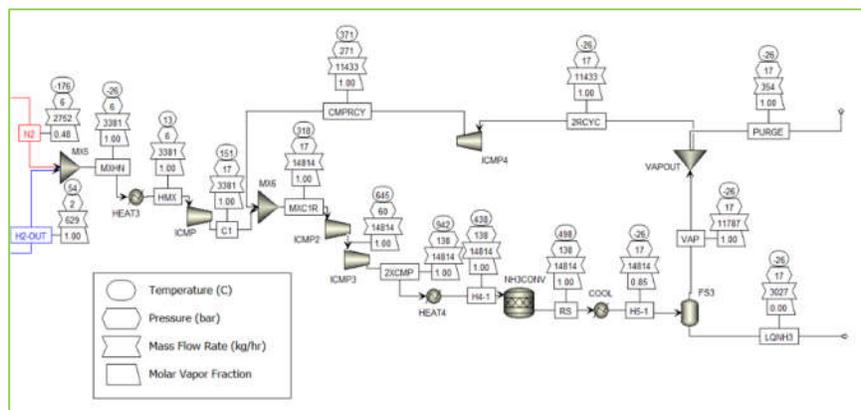
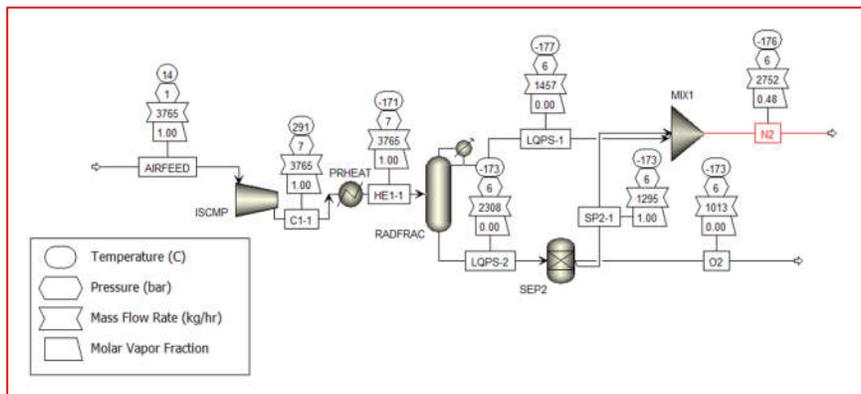


Figure 4. Detailed plant layout of the simulated IPA synthesis plant.



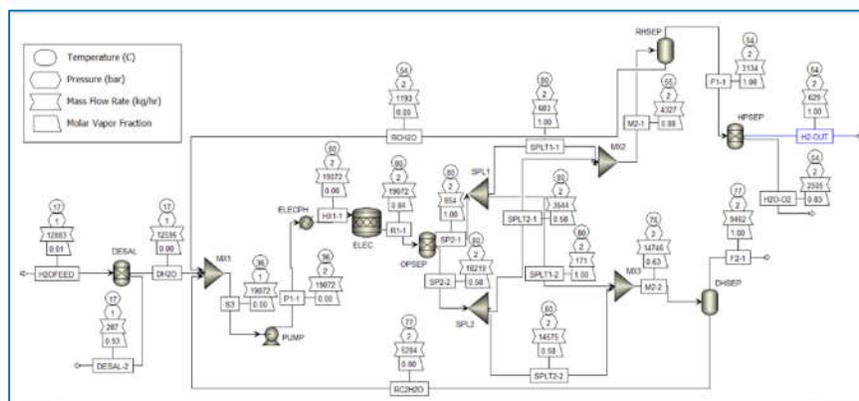


Figure 5. Clean NH₃ production flowsheet model. Three modules: hydrogen generation (blue), nitrogen generation (red), NH₃ synthesis (green). 'H₂-OUT' (blue) and 'N₂' (red) streams are input streams for the NH₃ synthesis module.

Table 1 shows the potential pathways that were identified via LCAs for each case study. The integrated FAHP-TOPSIS framework covers four criteria regarding IPA and green NH₃ production: technical, economic, environmental, and social. Each criterion has three sub-criteria that were specific to each case study (Tables 2-3) were derived based on prevalence and prominence throughout even relatively up-to-date literature [9,36,37]. Three sub-criteria per criterion was decided as the appropriate number; too few would be unusable in the MATLAB model, while too many would have increased the likelihood of data distortion, such as rank reversal). The literature review highlights an apparent lack of in-depth literature that explores the social dimension of holistically green sustainability over the past few decades, and even quite recently, despite the increasing awareness and necessity of holistically green sustainability. Therefore, the social (and by extension, the political) criteria for each case study has been expanded with a greater number of CPP-specific social sub-criteria for MCDM. This was based upon literature findings from Stojic et al. (2019), Fonseca et al. (2021), Guati-Rojo et al. (2021), and Kurien & Mittal (2022).

Table 1. Potential green and/or sustainable pathways for IPA synthesis and green NH₃ production.

Case study	Potential pathways
IPA via isopropyl acetate	<ol style="list-style-type: none"> 1. Direct Propylene Hydration (PH) 2. Propylene Indirect Hydration (IAH) Acetone Hydrogenation (AH)
Green NH ₃	<ol style="list-style-type: none"> 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)

Table 2. 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 3. Criteria and sub-criteria for green ammonia 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

3. Results

3.1. FAHP-TOPSIS

TOPSIS was applied to rank the IPA and green NH₃ production pathways. Because the pathway data has already been normalised and transformed into P_{ij} (Appendix E), further manual data processing was not required for the calculations in this section. Only the following sub-criteria weights were used in the ranking calculations: W_o , W_c , and W_i . Said sub-criteria weights were agreed to cover the overall encompassing ‘perspective’ of each pathway, in terms of holistically green sustainability. Tables 4 and 5 contains the results for the weight aggregation, that were derived from the results in Appendix F.

Table 4. All weight results by sub-criteria for the IPA synthesis pathways. A=Tech, B=Econ, C=Env, D=Soc.

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 5. All weight results by sub-criteria for the green NH₃ production pathways. A=Env, B=Econ, C=Soc, D=Tech.

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

D_i^+ and D_i^- represent the distances from the positive (Equation 11) and negative (Equation 12) ideal solutions, respectively, with $u=0.5$. Lower D_i^+ values denote smaller deviations from the positive-ideal solutions and consequently a higher-ranked pathway(s) (Xu et al., 2018). Therefore, IAH and HPEA are 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 does not consider the impacts of sensitivity analysis (Figures 6 and 7). Table 6 illustrates the distances for IPA and green NH_3 pathways.

Table 6. Distances from the positive and negative ideal solutions for each IPA (top) and green NH_3 (bottom) pathway. Combination, objective, and (comprehensive) subjective sub-criteria weights only.

	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
	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

Goodness-of-fit is the degree of fitness of each potential pathway to the D_i^- and D_i^+ values, in accordance with Equation 13. No significant deviations were apparent in the results of each weight type. Moreover, goodness-of-fit for the D_i^+ (C_i^+) appears to be in-line with the pathway rankings for each case study. Table 7 shows the goodness-of-fit, C_i^- and C_i^+ , for each potential pathway in IPA and green NH_3 production. Criterion weight (A-D) was altered at +0.1 increments, from +0 to +0.9, with a total of 40 variations with respect to the calculated C_i^+ values. Figures 6-7 show relative stability for each pathway respective of both case studies, with negligible change(s) in C_i^+ for W_i in response to criterion weight change.

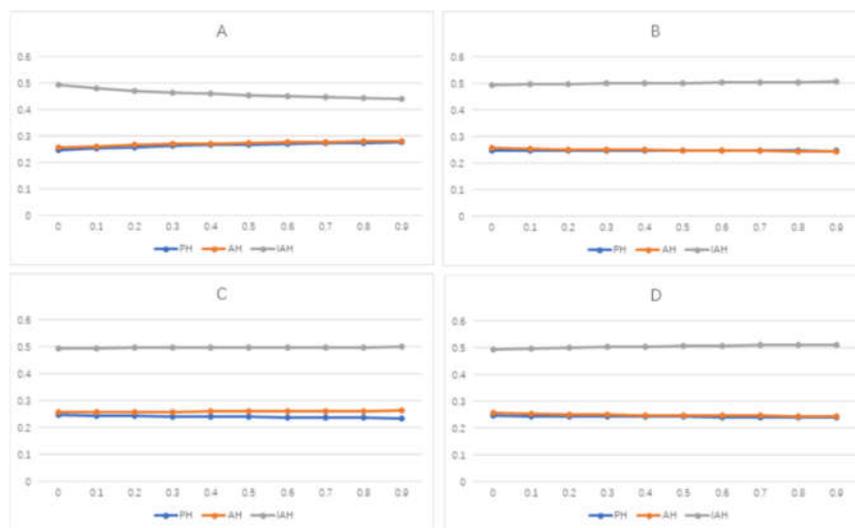


Figure 6. C_i^+ results relative to changes in technical (A; top-left), economic (B; top-right), environmental (C; bottom-left), and social (D; bottom-right) criterion weights for IPA pathways

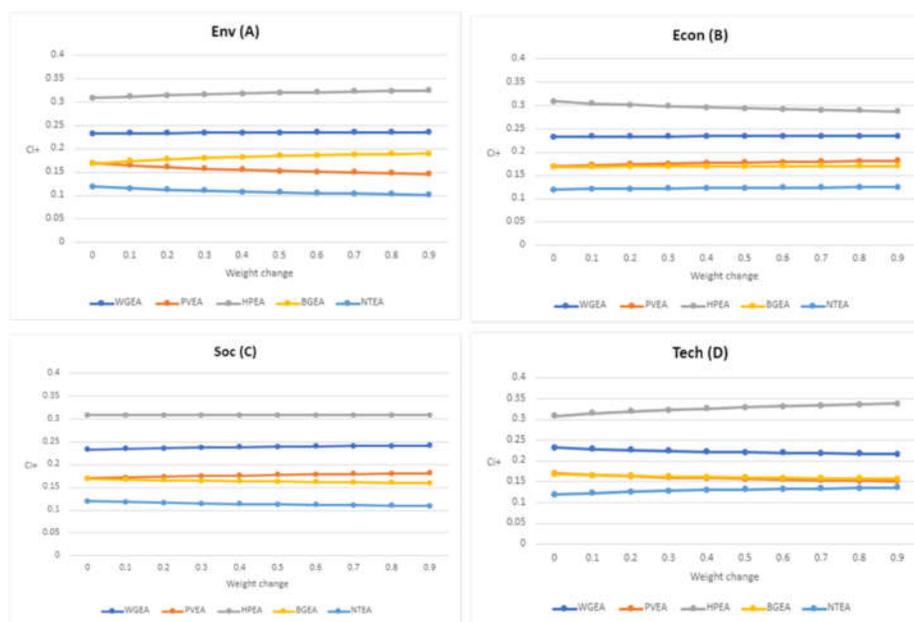


Figure 7. C_r^+ results relative to changes in environmental (A; top-left), economic (B; top-right), social (C; bottom-left), and technical (D; bottom-right) criterion weights for green NH_3 pathways

Table 7. Goodness-of-fit for each IPA (top) and green NH_3 (bottom) pathway. Combination, objective, and comprehensive subjective sub-criteria weights only.

	W_i		W_o		W_c	
	$C_{\bar{r}}$	C_r^+	$C_{\bar{r}}$	C_r^+	$C_{\bar{r}}$	C_r^+
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
	W_i		W_o		W_c	
	$C_{\bar{r}}$	C_r^+	$C_{\bar{r}}$	C_r^+	$C_{\bar{r}}$	C_r^+
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

3.2. Formatting of Mathematical Components

3.2.1. TOPSIS

$$A = (a_{ij})_{mn}, \quad (1)$$

In which the decision matrix, A , was calculated from $m =$ alternatives, with respect to n criteria; a_{ij} = intersection of each criterion and alternative [Equation 1].

$$r_{ij} = \frac{a_{ij}}{\sqrt{\sum_{k=1}^m a_{kj}^2}} \quad (2)$$

Equation 2 derived the normalised decision matrix, R , with the equation for r_{ij} , typically via vector normalisation ($i = 1, 2, 3, \dots, m; j = 1, 2, 3, \dots, n$).

$$T = (t_{ij})_{mn} \quad (3)$$

$$t_{ij} = r_{ij} * w_j \quad (4)$$

Equation 3 calculated the weighted normalised matrix, T via Equation 4. $i = 1, 2, 3, \dots, m; j = 1, 2, 3, \dots, n$. $w_j = j$ criteria weighting.

$$S^+ = \{\tilde{t}_1^+, \tilde{t}_2^+, \tilde{t}_n^+\} \quad (5)$$

$$S^- = \{\tilde{t}_1^-, \tilde{t}_2^-, \tilde{t}_n^-\} \quad (6)$$

The positive-ideal and negative-ideal solutions were derived via Equation 5 and Equation 6, respectively. Balioti et al. (2018) applies fuzzy logic, while the classical method applies crisp numbers.

$$D_i^+ = \sqrt{\sum_{j=1}^n (t_{ij} - t_j^+)^2} \quad (7)$$

$$D_i^- = \sqrt{\sum_{j=1}^n (t_{ij} - t_j^-)^2} \quad (8)$$

Equation 7 and Equation 8 calculated the distances of each alternative from the positive-ideal and negative-ideal solutions, D_i^+ and D_i^- , respectively.

$$C_i = \frac{D_i^-}{(D_i^+ + D_i^-)} \quad (9)$$

Equation 9 was used to derive the relative closeness, C_i ; '1' = positive-ideal, '0' = negative-ideal. Preference ranking order was created on C_i , in which max C_i represents the optimum alternative.

3.2.2. Weight calculations

$$f_{ij}(+) = \frac{f'_{ij} - \min(f'_{ij})}{(\max f'_{ij} - \min f'_{ij})} \quad (10)$$

$$f_{ij}(-) = \frac{\max(f'_{ij}) - f'_{ij}}{(\max f'_{ij} - \min f'_{ij})} \quad (11)$$

Where f_{ij} represents normalised data, and f'_{ij} represents original data for IPA and green NH₃ (Appendix G). And to ensure non-zero results for later logarithmic calculations, a constant C of 0.0001 is added to the normalised data (Appendix H).

$$P_{ij} = \frac{f_{ij}}{\sum_{i=1}^n f_{ij}} \quad (12)$$

$$e_j = -\frac{1}{\ln n} \sum_{i=1}^n (P_{ij} \ln P_{ij}) \quad (13)$$

$$g_j = 1 - e_j \quad (14)$$

$$W_o = \frac{g_j}{\sum_{j=1}^m g_j} \quad (15)$$

Characteristic proportions, P_{ij} , was calculated via Equation 12. Entropy value, e_j , and the coefficient of difference, g_j , of i -th object for each j -th (sub-)criterion were then derived via Equation 13 and Equation 14, respectively. n is the number of pathways/routes; $n=3$ for IPA, and $n=5$ for green NH₃. Equation 15 was applied to calculate W_o , where m was the total number of g_j values.

$$w_c = w_r w_s \quad (16)$$

$$w_i = \frac{(w_c)^u (w_o)^{1-u}}{\sum_{i=1}^n (w_c)^u (w_o)^{1-u}} \quad (17)$$

Comprehensive subjective weights (W_c) must also be calculated to determine the combination weights (W_i) that can be applied in TOPSIS. Equation 16 and Equation 17 are used to derive each set of weights, respectively, where $u=0.5$.

4. Discussion

The FAHP-TOPSIS framework optimises the decision-making process regarding IPA and green NH_3 production via pathway prioritisation, based on case-specific criteria and/or sub-criteria, from a holistically green and/or sustainable perspective. FAHP enabled the use of qualitative data via TFNs for criteria and sub-criteria weighting. TOPSIS was selected to rank the pathways, due to its relative stability, accuracy, and available model in MATLAB by Li et al. (2023). The “decision-makers” in this paper are regarded as a more homogeneous identity, primarily for the sake of ease and to focus on the MCDM framework. In real-life, the composition of decision-makers would be more explicitly diverse, from industry professionals to more business-orientated backgrounds.

IAH (0.250) and HPEA (0.180) were prioritised as the most optimal pathways, because they had the smallest D_i^+ values in W_i , for their respective case studies. Likewise, the least optimal pathways were identified as AH (0.551) and NTEA (0.388). Therefore, the most to least optimal pathways for IPA were IAH>PH>AH. However, there might be slight contention between the prioritisation of PH and AH, due to the closeness in D_i^+ values. The green NH_3 pathways were prioritised as follows: HPEA>WGEA>BGEA>PVEA>NTEA, in which the close D_i^+ values may also cause contentious ranking between BGEA and PVEA, particularly dependent on criteria and/or sub-criteria weighting. Overall, C_i^+ values for W_i aligns with this order of pathway prioritisation, in terms of balance and stability. And as it was highly recommended in the literature, sensitivity analysis (Appendices K-L) was thus carried out to evaluate the overall robustness of the FAHP-TOPSIS framework.

That said, there are uncertainties among sub-criteria by themselves and in relation to each other, especially in terms of potential changes over time. The degree of uncertainty could be attributed to a lack of access to reliable and accurate software, such as that for techno-economic analysis. Sub-criteria like NPV, policy applicability, and equipment costs 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 [49-51]. Model development is contingent on a relatively case-to-case basis, especially if it is designed to be optimised towards truly holistically green sustainability in any CPP.

Therefore, future works should seek to develop and implement a more robust and reliable framework for further overall optimisation; specifically, an integrated FAHP-VIKOR with PROMETHEE-II framework, with a more explicit integration of process systems engineering (PSE) tools, such as LCAs, LCCA, and social-LCAs. VIKOR, while similar to TOPSIS, has normalised values that are independent of the criterion's evaluation unit via linear normalisation instead of TOPSIS' vector normalisation [22,30]. Furthermore, VIKOR can provide a more reliable representation of decision-maker viewpoints via compromise solutions without data distortion [30], especially as closeness to the ideal solution may not equate to the most ideal solution(s) [22]. PROMETHEE-II is a popular MCDM method in green sustainable research fields, because it allows for a complete ranking of alternatives [22,36,39]. Additionally, 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 [23,38]. FAHP would provide the appropriate criteria and sub-criteria weightings via decision-makers, which mitigates one of PROMETHEE's key potential weaknesses; questionably reliable criteria/sub-criteria weighting [25,31].

5. Conclusions

The FAHP-TOPSIS framework serves to validate the implementation of an integrated MCDM framework for prioritising holistically green IPA and NH_3 production pathways. However, data must be clearly processed to maximise the understanding and effectiveness of the FAHP-TOPSIS

framework. According to the D_i^+ and C_i^+ values (Tables 6-7), the most to least optimal pathway 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 pathway for green NH₃ is as follows: HPEA>WGEA>BGEA/PVEA>NTEA. Said orders of pathway prioritisation is further validated via sensitivity analysis for each criterion, which show negligible changes in C_i^+ relative to weight change (Appendices K-L) and thus a robust MCDM framework. Moreover, the C_i^+ values for W_i aligns with this order of pathway prioritisation, from a more balanced and stable perspective. However, while the MCDM results can provide an overall perspective in respect to each criterion, there are 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.

Nevertheless, the FAHP-TOPSIS framework demonstrates that MCDM can implement greater optimisation within chemical process plants (CPPs) via pathway prioritisation based on holistically green and/or sustainable, case-specific criteria and/or sub-criteria. Future research would seek to develop a more comprehensive sustainability governance platform. This would involve the systematic integration of process systems engineering (PSE) tools—(life-cycle assessments (LCAs), social-LCAs, and life-cycle cost analysis (LCCA)—via Sima Pro with an integrated MCDM framework (FAHP-VIKOR with PROMETHEE-II). The improved methodology framework will further validate the employment of integrated MCDM frameworks for various CPPs. VIKOR would provide a more reliable representation of decision-maker viewpoints, with minimal data distortion, and possible compromise solutions. PROMETHEE-II is commonly applied in green sustainable research fields, as it allows for a complete ranking of alternatives with a relatively high level of stability and reliability. Furthermore, decisive results can be derived with/without grey data, and without the requirement of data normalisation, unlike TOPSIS.

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Abbreviations

The following abbreviations are used in this manuscript:

MDPI	Multidisciplinary Digital Publishing Institute
DOAJ	Directory of open access journals
TLA	Three letter acronym
LD	Linear dichroism

Appendix A

Table A1. Linguistic-based fuzzy comparison matrix of crisp AHP values to TFNs [38].

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

Appendix B

Table A2. First-layer (i.e., the criteria) subjective pairwise comparison matrix for IPA synthesis. 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 A3. First-layer subjective pairwise comparison matrix for green NH₃ production. REI, RV, and RF are the reciprocals of EI, V, and F, respectively.

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

Appendix C

Table A4. Fuzzy judgements converted into TFNs with the CR, subjective criteria weights (W_r), and fuzzy synthetic extent values, S.

	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
							0.122
B	(5/2,3,7/2)	(1,1,1)	(1,3/2,2)	(2,5/2,3)		0.402	0.272
					0.408		

						0.596
						0.188
C	(2,5/2,3)	(1/2,2/3,1)	(1,1,1)	(1,3/2,2)	0.290	0.289
						0.439
						0.119
D	(1,3/2,2)	(1/3,2/5,1/2)	(1/2,2/3,1)	(1,1,1)	0.185	0.182
						0.282

Appendix D

Table A5. Fuzzy judgement matrix for criterion A, where W_s = subjective sub-criteria weight.

A	A1	A2	A3	CR	W_s	S
A1	(1,1,1)	(3/2,2,5/2)	(1/2,2/3,1)		0.372	0.247
						0.373
						0.570
A2	(2/5,1/2,2/3)	(1,1,1)	(1/2,2/3,1)	0.0873	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 A6. Fuzzy judgement matrix for criterion B.

B	B1	B2	B3	CR	W_s	S
B1	(1,1,1)	(3/2,1,2)	(1/2,2/3,1)		0.418	0.250
						0.421
						0.667
B2	(1/2,1,3/2)	(1,1,1)	(3/2,1,2)	0.0566	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 A7. Fuzzy judgement matrix for criterion C.

C	C1	C2	C3	CR	W_s	S
C1	(1,1,1)	(3/2,1,2)	(3/2,1,2)		0.489	0.324
						0.492
						0.723
C2	(1/2,1,3/2)	(1,1,1)	(1/2,2/3,1)	0.0455	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 A8. Fuzzy judgement matrix for criterion D.

D	D1	D2	D3	CR	W _s	S
D1	(1,1,1)	(1,3/2,2)	(3/2,2,5/2)		0.454	0.288 0.458 0.696
D2	(1/2,2/3,1)	(1,1,1)	(1,3/2,2)	0.0349	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

Appendix E

Table A9. Characteristic proportion, P_{ij} , values for the IPA pathways.

	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 A10. Characteristic proportion, P_{ij} , values for the the green NH₃ pathways.

	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	0.5384	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

Appendix F

Table A11. e_j , g_j , and W_o results for each sub-criterion for the IPA synthesis pathways.

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	0.500	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 A12. e_j , g_j , and W_o results for each sub-criterion for the green NH_3 pathways.

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	

Appendix G

Table A13. Original 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 A14. Original data for the five green NH₃ 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

Appendix H

Table A15. Normalised data for the IPA pathways.

Constant added +0.0001	PH	AH	IAH
A1 (+)	0.577	0.0001	1.0001
A2 (+)	0.5001	1.0001	0.0001
A3 (+)	1.0001	1.0001	0.0001
B1 (-)	0.586	0.0001	1.0001
B2 (+)	0.0001	1.0001	1.0001
B3 (-)	0.314	0.0001	1.0001
C1 (-)	0.0001	0.600	1.0001
C2 (-)	0.580	0.0001	1.0001
C3 (+)	0.0001	1.0001	1.0001
D1 (-)	0.0001	0.5001	1.0001
D2 (+)	0.0001	0.0001	1.0001
D3 (+)	1.0001	0.5001	0.0001

Table A16. Normalised data for the green NH₃ pathways.

Constant added +0.0001	WGEA	PVEA	HPEA	BGEA	NTEA
A1, kg (-)	0.151	0.0931	0.954	1.0001	0.0001
A2, kg CO ₂ eq (-)	0.796	0.0001	1.0001	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	1.0001	0.109	0.171975	0.0001
B3, % (+)	0.552	0.263	1.0001	0.0001	0.154
C1, scores (-)	1.0001	1.0001	1.0001	0.485	0.0001
C2(+)	1.0001	1.0001	0.820	0.355	0.0001
C3(+)	0.742	0.522	1.0001	0.0001	0.0001
D1, % (+)	0.210	0.0001	1.0001	0.180	0.433
D2 (+)	0.455	0.0001	1.0001	0.0001	0.455
D3 (+)	0.314	0.314	1.0001	0.418	0.0001

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