D14.1 Materials properties suitable for Unit 1 (draft)

Project Information	
Title	From solar energy to fuel: A holistic artificial photosynthesis platform for the production of viable solar fuels
Acronym	REFINE
Project Call	HORIZON-CL5-2022-D3-03
Project Topic	HORIZON-CL5-2022-D3-03-03
Grant Agreement ID	101122323
Project Duration	48 months: 1st November 2023 – 31st October 2027

Document Information	
Contractual Date of Delivery	M12
Actual Date of Delivery	M12
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Contributing Participant(s)	UiO, IFE, AUTH
Work Package(s)	WP14
Dissemination Level (PU/SEN)	PU
Nature (R/DEC/DEM/DMP)	R
Version	1.1

This project has received funding from the European Union HORIZON Research and Innovation Actions under grant agreement ID 101122323

Document History

Version	Issue Date	Changes
[1.0]	30.10.2024	
[1.1]	11.11.2024	Revised version. Added disclaimer text on page 45

Table of Contents

1 Summary and scope

Work Package 14 (WP14) comprises of three key undertakings where the first involves the application of a Multi-Criteria Decision Analysis (MCDA) to aid in the selection of materials and configurations of Unit 1. An overview of the REFINE process recognises two key units with the first containing the photovoltaic and electrolytic devices. These have emerged as critical technologies within the renewable energy industry and are combined in the purposes of REFINE to deliver the input stream of green hydrogen for Unit 2.

Material selection is necessary to support decisions made by the technical teams associated with Unit 1 by comparing design options using detailed guidelines. Technical performance considers static and dynamic properties as well as the composition and scale of throughputs which ensures that the selected options can withstand operating (mechanical, chemical, electrical etc.) and external stresses. Additionally, this process adds another level of robustness by assessing further design metrics which do not necessarily impact material function, but should still be considered: including cost-effectiveness, safety (to humans and wildlife) and overall lifecycle performance.

In conducting this analysis, the principal aim is to identify optimal recommendations in the design of Unit 1 components consistent with sound technical performance and commitments to sustainability. Sustainability is examined from three perspectives: environmental, economic and social which evaluate the reasons outlined above driving the material selection process. We apply further consideration to other sustainability models including the Circular Economy framework to apply the sustainability domains to various stages of the materials' life cycle.

The completion of this report highlights the collaborative efforts of multiple REFINE members associated with the Unit 1 devices as well as WP14, however the conclusion will highlight how the final draft can incorporate more expertise.

1.1 Objectives

As highlighted, the MCDA aims to provide a recommendation for the assessed Unit 1 components by using the following objectives which are expanded from the material selection process.

1. **Identify MCDA Application Areas:** Determine components and design elements involved with the PV module and electrolyser where an MCDA is required i.e. decisions where there is more than one option being considered.

2. **Develop Relevant Criteria:** Establish a comprehensive set of criteria within the technical, environmental, economic and social domains that address key challenges and performance targets outlined by the technical teams.

3. **Conceive Evidence-Based Recommendations:** Provide valid recommendations supported by a multi-criteria decision analysis using peer-reviewed literature, public records and reliable industry sources.

2 Multi-Criteria Decision Analysis (MCDA): Application and Method

Multi-Criteria Decision Analysis (MCDA) describes a category of methods for complex decision-making processes to assess options from a large set of guidelines [1]. Although there are various MCDA approaches, the Analytic Hierarchy Process (AHP) was employed in the material selection to provide simple and logical arguments for arriving at the recommendations detailed in the results [2]. This methodology is further benefitted by its versatility which easily accommodates multileveled weightings from the domains and sub criteria as well as the range of quantitative and qualitative factors simultaneously. The general structure of the AHP uses the following the stages:

1. Describe the issue and determine the aim
2. Structure the hierarchy by assessing three stages:
    - ***Domain:*** e.g. Technical, Environmental, Economic and Social
    - ***Criteria:*** e.g. Tafel Slope, Recyclability, Capital Cost and Human Toxicity etc.
    - ***Alternatives (Materials/Configuration):*** *e.g.* Ni Mesh, STF, IBC Cells etc.
3. Apply weightings to the Domains and Criteria with considerations to the aim
4. Define a ratio scale for each criterion (0-5 etc.) and apply the scores
5. Calculate the overall scores using the weightings and identify the top scoring options

The overview of the stages display the ease of applying this method to our material selection process. Its versatility with criteria type, multileveled decision making (i.e. recommend options via overall, domain or criteria score) and application of a ratio scale for scoring makes this analysis easy to conduct and track results from.

2.1 2.1 Scope

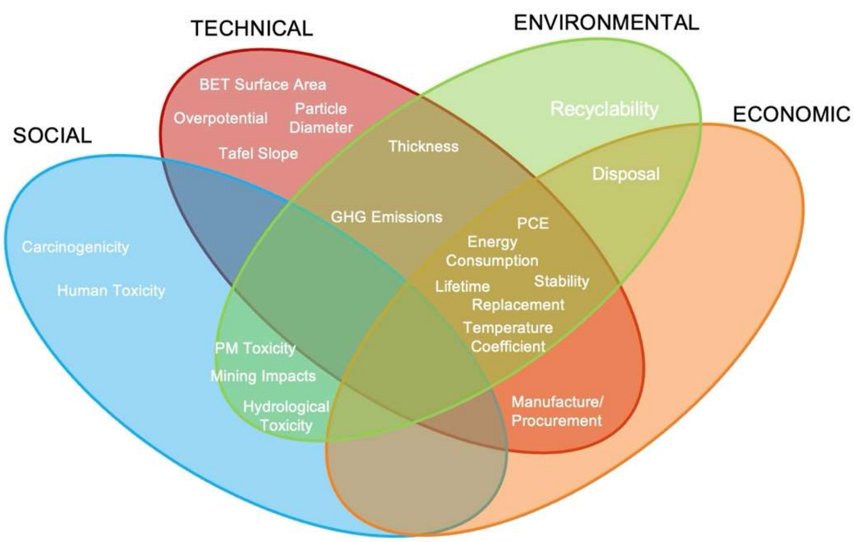

Figure 1: Overlapping MCDA Domains for Defining Sub-criteria.

A critical component of the material selection process is with identifying the specific application requirements and performance needs of the design elements. These requirements shape the scope by mutually identifying what factors necessitate consideration (i.e. our domains: technical, environmental, economic and social) and therefore the criteria derived from these characteristics. Figure 1 illustrates the overlap between these influences and demonstrates how an individual criterion can constitute a combination of these and how criteria selection must have clarity within their definitions to ensure uniqueness.

Another area where we must define our scope is with the identification of the Unit 1 components which require material selection. From consultation with the technical teams, these were found to be the anode and cathode catalysts and substrates and the cell configuration of the PV module. Although Unit 1 comprises of numerous components which are suitable for material selection analysis, these design elements were prioritised due to their significant impact to the overall performance and output of the system.

Lastly, the scope defines at which lifecycle stage each criterion has been applied. While this study evaluates materials for equipment design rather than a final manufactured product, factoring this with the analysis is appropriate since:

1. The selected materials will eventually require replacement and disposal so manufacture and End-of-Life (EoL) stages should be considered
2. Many of the materials assessed for application within the electrolyser components are not commercial and have been specifically synthesised by REFINE members which offers the opportunity to further assess manufacture procedures or compositions from the outset
3. Early intervention in the material development stage allows for the integration of circular economy principles, including selection of sustainable raw materials or implementation of lower energy consumption synthesis routes

The tables in the next section define each of the assessment criteria and describe the lifecycle stage this was applied to. We see that there is a trend in applying the criteria to predominantly the raw material extraction and manufacturing phases which highlights the value of this consideration due to the additional support we can provide to the technical teams involved in the synthesis of these materials.

2.2 Domains and Criteria Selection

To create a more rigorous methodology and comply with the research purposes outlined in the objectives, consideration should be applied to non-technical standards as well. These are identified within a sustainability framework which refers to the environmental, economic and social aspects which scrutinise options outside of performance expectations. Within these domains, supplemental criteria have been derived to represent a mix of the key issues and concerns within that individual group. Below denotes the criteria we considered under this framework along with their definitions and explained applications within the MCDA for the PV cell and electrolyser. Technical criteria will be explored further ahead as these have been independently selected for each subunit and components.

Environmental

This domain addresses some of the key issues that are most commonly reported to impact the environment, including: resource depletion, pollution, greenhouse gas emissions, circular economy, impact to the ecosystem and waste generation. Although, there are other issues that require assessment, such as water consumption or biodiversity impact, reporting on these for our observed materials are fairly limited and difficult to derive reliable comparative scorings for so these have not been considered under this assessment. However, since a life-cycle assessment will be conducted as one of the tasks for WP14, these issues will be addressed then.

Table 1: Environmental Criteria Definitions and Scoring Metrics

Criterion	Definition	Life Cycle Scope	Unit	Scoring Method
Lifetime	The operational life of the material or configuration before reported degradation/reduction to efficiency where the impact of continued use produces an unsafe environment or impact to production is significant enough to require replacement.	Use	Hours	0 – Option has a very short lifetime and requires replacement frequently within 10-year period i.e. 3 or more times. 1 – Option demonstrates moderate-low durability lasting between 4-7 years and requiring replacement at most twice within 10-year period. 2 – Option demonstrates moderate durability lasting 8-11 years (over 10 year period assessed for replacement requirement) 3 – Unreported information. 4 – Option demonstrates moderate-high durability lasting 12-15 years (over 10 year

				period assessed for replacement requirement) 5 – Option demonstrates high durability lasting over 15 years without replacement requirement due to no detectable degradation to performance.
GHG Emissions	The GHG emissions associated with the manufacture of the materials or configurations. This considers the CO_2 equivalence of all greenhouse gases involved.	Raw material extraction and Manufacturing for electrolyser Manufacturing for PV cell	kg CO2e	0 – Process for manufacture of option uses highest temperatures than other options and requires multiple processing steps i.e. >10 steps. 1 – Process for manufacture of option now uses high temperatures and requires a few more processing steps i.e. <10 steps. 2 – Process for manufacture of option now uses moderate temperatures but requires a few more processing steps i.e. <10 steps. 3 – Unreported information. 4 – Process for manufacture of option still uses lower temperatures than other options but requires a few more processing steps i.e. <10 steps.

				5 – Process for manufacture of option uses significantly lower temperatures than other options or much shorter processing steps i.e. <5 steps.
Particulate Matter Toxicity	Whether the materials involved in the composition or configuration are listed as monitored inhalable particulates in the UK and are considered as a pollutant or adverse to human health i.e. described as PM_{10}. This further considers measured concentrations and comparison to EU limits of 50 mg/m^3 for general PM_{10} contaminants or 20 ng/m^3 specific to Ni particulates.	Raw material extraction, manufacture and disposal/recycling	ng/m^3	0 – Contains at least 1 material that is reported to be over the EU limits or 4+ materials currently being monitored but under the EU limits. 1 – Contains 3 materials currently being monitored and are all reported in the UK as under the EU limits. 2 – Contains 2 materials currently being monitored and are all reported in the UK as under the EU limits. 3 – Unreported information. 4 – Contains 1 material currently being monitored and is reported in the UK as under the EU limits. 5 – Materials in configuration are not monitored as they do not present as current concern.
Hydrological (soil-based) Toxicity	Whether the materials involved in the composition or configuration are listed as monitored heavy metals or metalloids contaminating soils in UK. Their current measurements are used	Raw material extraction, manufacture and disposal/recycling	g/kg	0 – Contains at least 1 material that is reported to be over the EU limits or 3+ materials currently being monitored but under the EU limits.

	to compare with the WHO's permissible limits.			1 – Contains 3 materials currently being monitored and are all reported in the UK as under the EU limits. 2 – Contains 2 materials currently being monitored and are all reported in the UK as under the EU limits. 3 – Unreported information. 4 – Contains 1 material currently being monitored and is reported in the UK as under the EU limits. 5 – Materials in configuration are not monitored as they do not present as current concern.
Recyclability	This criterion considers the material which forms the bulk of the structure for the electrolyser options, but overall configurations for the PV cell. This explores whether material/s can be recycled for initial purpose, alternative purpose or must be disposed of altogether.	Disposal/recycling	Number of Cycles, Ease of Recycling	0 – Option is single use and must be disposed after / cannot be recycled or repurposed. 1 – Option contains mostly materials which can be repurposed for a lower value use. 2 – Option contains a proportional or slightly greater composition of non-100% recyclable materials. 3 – Unreported information.

	4 – Option is 100% recyclable or contains mostly 100% recyclable materials but is less easy/widely recycled. 5 – Option is 100% recyclable and reported to be easily or widely recycled.

Economic

Some of the concerns highlighted below touch on the issues addressed in the environmental domain which include stability (i.e. lifetime) and raw resources. We consider cost at four tiers of the life cycle: extraction, manufacture, use and disposal. Although, this covers the full life cycle; this does not consider alternative economic factors which may relate to some of the current options; these include transportation/logistical or other maintenance associated costs. Due to the novelty of some materials and difficulty in finding clear costs in other options, only a few economic issues have been considered at this time, but this will be further developed during the techno-economic analysis (TEA).

Table 2: Economic Criteria Definitions and Scoring Metrics

Criterion	Definition	Scope	Unit	Scoring Method
Capital cost	Relating to the electrolyser, this considers the cost of individual materials in the composition as a cost per bulk weight i.e. no consideration of synthesis method. Concerning the PV cell, this considers the cost of manufacturing by equating cost to a unit of output produced.	Raw material extraction for electrolyser Raw material extraction and manufacture for PV cell	EUR/kg EUR/W	0 – Option uses all high-cost resources and a complex and high-energy extensive processing procedure leading to overall cost greater than EUR10^5. 1 – Option uses mostly high-cost resources and a complex or high-energy extensive processing procedure leading to overall cost within EUR10^5. 2 – Option uses a mix of low-cost and high-cost resources paired with a moderately complex or mid-energy extensive processing procedure leading to overall cost within EUR10^4. 3 – Unreported information.

				4 – Option uses mostly low-cost resources or a somewhat simple or low-energy extensive processing procedure leading to overall cost (e.g. within EUR10^3) 5 – Option uses abundant and very low-cost resources or a simple and low-energy extensive processing procedure leading to overall cost (e.g. within EUR10^2)
Replacements	The cost of maintaining the material or configuration within a 10 year period exclusively considering only replacements instead of the potential for repairs. This criterion ties in with the lifetime found for each option and is associated alongside the from this and the costs found from t	Up to use	EUR/10-Years	0 – Option is a mix of very low cost and lifetime. 1 – Option is a mix of low cost and lifetime. 2 – Option is a mix of moderate cost and moderate lifetime. 3 – Unreported information. 4 – Option is low cost, and high lifetime i.e. may score 4 or 5s for each category. 5 – Option is very low cost, and very high lifetime i.e. scores top in each category.
Disposal/Treatment	The cost of the disposal process associated with the material or contaminants within the option. The ratio of non-hazardous to hazardous contaminants is observed and ranked	Disposal and recycling	EUR	0 – Option contains mostly or all hazardous waste and is difficult to recycle or dispose/requires specialised treatment centres.

	to be associated with higher cost with options containing more hazardous compositions.			1 – Option contains mostly hazardous waste and is difficult to recycle or dispose. 2 – Option contains proportional amounts of hazardous and non-hazardous waste and is moderately difficult to recycle or dispose. 3 – Unreported information. 4 – Option contains mostly non-hazardous waste and is recycled or disposed of widely. 5 – Option does not contain any hazardous waste and is recycled or disposed of widely.

Social

Considering the social implications of the recommendations from the study are critical in understanding the impact to people and communities. Likewise, with economic factors, social criteria are also interlinked with some key environmental issues particularly with harm to wildlife either due to direct hazards with the material or of land-use. This domain expands on key social issues expanding across the materials' life cycle which include ethics, human rights and community welfare.

Table 3: Social Criteria Definition and Scoring Metrics

Criterion	Definition	Scope	Unit	Scoring Method
Human Toxicity	Explores the potential of a metal, chemical or substance to cause harm to human health through any exposure route leading to mild or severe effects occurring immediately or over a longer period. These have been cross referenced with medical resources and safety data sheets (SDS) as causes for concern.	Manufacture	Number of toxic contaminants	0 – Contains or involves 4+ materials/metals which are known to be harmful. 1 – Contains or involves 3 materials/metals which are known to be harmful. 2 – Contains or involves 2 materials/metals which are known to be harmful. 3 – Unreported information. 4 –Contains or involves 1 material/metal which is known to be harmful. 5 – Does not contain or involve any materials/metals which are known to be harmful.
Carcinogenicity	Considers the ability of any involved materials to cause cancer in humans from a range of exposure times. Distinguishes scores based on known,	Manufacture	Carcinogen Groups	0 – Contains or involves at least 1 known carcinogen and >2 probable/possible carcinogens

	probable and possible carcinogens from each step of the life cycle which involves exposure to the material.			1 – Contains or involves at least 1 known carcinogen. 2 – Contains or involves up to materials/metals which are probable carcinogens. 3 – Unreported information. 4 –Contains or involves material/metal which are possibly carcinogenic. 5 – Does not contain or involve any materials/metals which are known to be carcinogenic.
Mining Implication	This explores ethical issues associated with the extraction of the raw materials used to construct each of the considered alternatives. The issues explored include child labour, unsafe work conditions and impact to the mined area. Consideration to these sub-parameters were used since these were identified in the report as some of the key shared ethical offences in industrial materials. The method of scoring involves breaking down the raw materials involved in the composition or configuration of each option and matching this to the list of materials reported in the study. These materials were assessed to find which of the ethical offences they violate. An example is seen in Table 4, Option 1	Raw material extraction	See table below	0 – Contains 6+ materials/metals which are involved in any of the mining issues in Table 4. 1 – Contains 5-6 materials/metals which are involved in any of the mining issues in Table 4. 2 – Contains 3-4 are materials/metals which are involved in any of the mining issues in Table 4. 3 – Unreported information. 4 – Contains 1-2 materials/metals which are

	contains 2 materials which have been found to use child labour, 3 materials which violate unsafe work conditions and 1 material which has grievous impact to the mined area giving this a total sum of offences as 6. Scores have been applied from the value of these summed offences.		involved in any of the mining issues in Table 4. 5 – Does not contain any materials/metals which are involved in any of the mining issues in Table 4.

Table 4: Example Tally for Mining Impact Assessment

Option	Child Labour	Unsafe Working Conditions	Grievous Impact to Mined Area	Sum
1	2	3	1	6
2	1	2	1	4
n	x	y	z	x+y+z

Technical: Electrolyser

The scores for the technical criteria are less specific to those described for the previous domains. These are more standard and general where 0 – Very Poor, 1 – Poor, 2 – Moderate, 3 – Unreported Information, 4 – Good and 5 – Very Good.

Table 5: Electrolyser Catalyst Technical Criteria

Criterion	Definition	Unit	Relevance
BET Surface Area	BET (Brunauer-Emmett-Teller) surface area measures the specific surface area of a material by	m^2/g	• Can allude to the catalytic activity of the material • Larger surface areas increase the number of contact points for chemical reactions

	quantifying the total surface area per its unit mass.		
Particle Diameter	Particle diameter refers to the size of the catalytic active sites.	μm	• Can indicate the catalytic activity of a material as smaller particle diameters have higher surface:volume ratios • Can indicate the stability of a catalyst – larger particle sizes may indicate sintering meaning catalyst degradation
Electrical Conductivity	Electrical conductivity measures the ability of the material to conduct electric current.	S/cm	• High electrical conductivity indicates good electron transfer which is required to drive electrochemical reactions • This also indicates lower power losses from reduced electrical resistance
Overpotential	Overpotential is the difference in the theoretical vs applied potential (voltage) required to drive a half-cell reaction at an electrode to achieve a certain rate.	mV	• Low overpotential indicates high electrochemical efficiency as less excess energy is required alongside the theoretical potential • This also indicates faster reaction kinetics where higher reaction rates can be achieved
Tafel Slope	The Tafel slope indicates how the overpotential changes with significance to the current density.	mV/dec	• Low Tafel slopes indicate fast reaction kinetics and higher rates of electron transfer • This indicates good catalytic performance since faster rate of reaction are achieved

Technical: PV Cell

The scores for the PV module match those used for the electrolyser elements where 0 – Very Poor, 1 – Poor, 2 – Moderate, 3 – Unreported Information, 4 – Good and 5 – Very Good.

Table 6: PV Module Technical Criteria

Criterion	Definition	Unit	Relevance

Power Conversion Efficiency (PCE)	PCE is the percentage of light energy that can be converted into electrical energy by a PV cell.	%	• A high PCE indicates increased efficiency and productivity of the output power produced • Less energy is wasted via heat or other forms as a higher proportion of the input energy is converted to the desired output
Stability	Stability refers to the ability of the PV cell to maintain its performance over time under various operating conditions.	Hours/ Qualitative	• Long-term stability indicates better performance over time where a high PCE can be maintained • This indicates reliable power output and is more economically beneficial as less replacements are required
Energy Consumption	This normalises the energy consumed during the manufacturing stage of a PV cell to create one unit of power.	kWh/kW	• Lower energy consumption is desired as it can lead to a higher net energy output (when considering energy consumption from manufacture) • This also leads to a smaller environmental impact as less resources are required
Thickness	Thickness refers to the physical dimension of the silicon wafer used in the PV cell.	µm	• Higher thickness impacts material usage and subsequent cost so a thinner wafer is preferred
Temperature Coefficient	In our application, the temperature coefficient quantifies the impact of the temperature to the PCE.	%/°C	• A lower temperature coefficient indicates better performance stability across a higher range of environmental conditions • Energy production is more consistent and reliable

2.3 Domain and Criteria Weightings

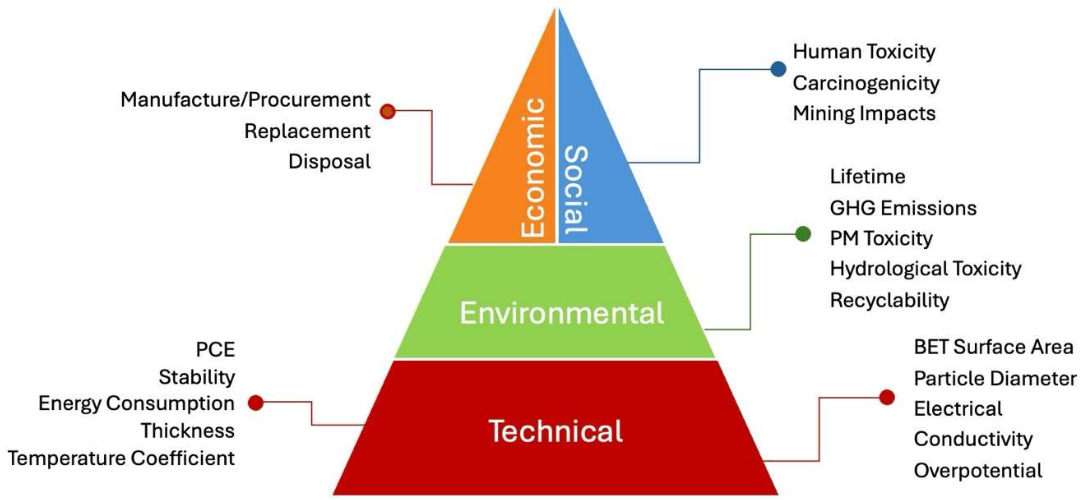

Figure 2: Hierarchy of Domains Associated with their Weightings.

Table 7: Justifications of Domain Weightings

Domain	Weighting (%)	Explanation
Technical	35	The primary function of the materials and configurations is to perform effectively in its intended role. The technical parameters reflect this the most and is therefore weighted the highest. Additionally, the criteria representing this domain, has been devised with other REFINE members outside of WP14 so this validates their importance to the overall objectives.
Environmental	25	Environmental concerns have a growing importance in the larger context outside of REFINE but is also one of the key driving forces for the emergence of WP14. This domain is ranked the second highest since it encompasses some key objectives between REFINE and WP14 which are heavily focused on green and environmentally driven purposes, goals and choices. This is ranked higher than the last two only marginally since it has more direct relevance to WP14.
Economic	20	Economic and Social criteria have been weighted the lowest and equal to each other at 20%. Although these are important factors that deserve consideration, they are secondary to the purposes of REFINE and WP14 in that their impacts are less direct to the performance of Unit 1. Additionally, much of the scorings applied with these criteria are more qualitative in nature and cannot be accurately measured without more comprehensive analysis methods i.e. expert surveys, TEA etc.
Social	20	

Inter-Domain Weightings

The bulk weightings assigned to the sustainability domains (environmental, economic and social) are equally divided between the criteria within each of these parameters. However, since we establish the importance of the technical variables, the weightings of these have been differentiated to prioritise dynamic metrics as detailed below.

The technical criteria assigned to the PV cell are weighted as shown in Table 8. This shows that ***Thickness*** and ***Energy Consumption*** are weighted equally less than the other parameters since these are less relevant to the performance of the PV cell and are potentially more applicable to sustainability considerations.

Table 8: Technical Criteria Weightings: PV Cell

Thickness	Energy Consumption	PCE	Stability	Temperature Coefficient
17.0	17.0	22.0	22.0	22.0

Thickness relates to the Silicon wafer layer of the PV cells and have been advised by the technical team as an important factor to consider when comparing the quantity of silicon used between the PV cell options. This pertains potentially more to environmental concerns with raw material usage as well as economic with cost considerations since this material comprises the bulk used in constructing the cells. Additionally, the values found for this criterion are fairly similar across the options, so scores reflect miniscule differences. For ***Energy Consumption*** this follows similar logic as before where this criterion pertains more to environmental concerns. Although this analyses the manufacturing stage of the options' lifecycles, this does not really have an impact to the function of the PV system.

Likewise with the electrolyser, Table 9 shows the allocation of the weightings between the indicators used to assess technical performance. This reveals that ***BET Surface Area*** and ***Particle Diameter*** influence less of the overall score pertaining to this domain.

Table 9: Technical Criteria Weightings Electrolyser

BET Surface Area	Particle Diameter	Electrical Conductivity	Overpotential	Tafel Slope
17.0	17.0	22.0	22.0	22.0

These parameters have reduced weightings since they are not directly relevant to the electrochemical performance of the materials but have still been considered since they allude to catalytic activity and stability. ***BET Surface Area*** and ***Particle Diameter*** are important to factor catalytic considerations however they are not categorically intrinsic with the materials since these are more influenced by the synthesis route selected to manufacture the options, so values observed in literature can vary greatly due to the experimental procedure.

2.4 Assumptions and Limitations

Table 10: Methodology Assumptions, Limitations and Improvements

Assumption	Limitations	Advised Improvements
A limited number (3-5) criterions chosen for each domain.	1. Disregard of more relevant or necessary criteria leading to misrepresentation or incomplete picture of the full domain.	Addition of more criteria to each of the domains. Consult technical teams to include updated parameters required to be studied.
	2. Oversimplification may have led to missing more complex or new/emerging sustainability concerns.	Review the criteria periodically before the final draft and include any new considerations from similar literature.
	3. Inviting personal or disciplinary biases with considering concerns most relevant to their work package objectives/interests.	Establish a diverse review panel to validate the work before the final submission. Create questionnaires/surveys to add/update criteria as advised by technical teams.
	4. Insufficient granularity between criteria which overlap in covering similar issues.	Reassess definitions to ensure detailed distinction between similar criteria. If any overlapping criteria is found, resolve this by eliminating one or applying distinct definitions to each.
	5. Reduced sensitivity to significant differences between material or configuration options due to missed considerations.	Develop detailed scoring metrics with current criteria and if scores or applied definition drift from what is presented in the methodology, consider this as a new parameter.

Weightings were decided between WP14 project members and have been distributed between domains and criterions from group discussions.	1. Inviting personal or disciplinary biases from less-technically involved REFINE members.	Corroborate with expert opinion from technical teams and outline the rationale behind updated weightings. Apply sensitivity analysis by using different weighting combinations.
	2. Limited perspective and diverse expertise from more knowledgeable REFINE members.	Include more comprehensive peer reviewing in the final draft to find gaps in justification of weightings.
	3. Justification for the recommendations may be more difficult to prove since weightings may be skewed and less credible.	Present the results transparently by referencing each reported value used for scoring. Ensure application of the scoring descriptions to avoid potential misrepresentations here.
Scores are explained for each criterion however 3 is defined for all as 'Unreported' regardless of whether all values for the options within the criteria are reported and known.	1. Falsely devalues some options where these have very minute differences to others	Consult with other members to uncover if this will have a significant impact to the final scores if maintained. Ensure that all criteria have detailed guidelines for the scores and any instances where this differs has been described and justified i.e. assumptions and limitations.
	2. Falsely inflates the overall scores of some materials more than others due to unreported information.	Compare with other missing data protocols used in other material selection analyses and validate applicability to this study.

Table 11: Domain Assumptions, Justifications and Limitations

Domain	Assumption	Justifications and Limitations
Environmental	Lifetime criteria scored for anodic catalyst options were estimated from the assessment of the stability of the A-site elements.	Lifetime is a difficult criterion to analyse as most testing is done under lab conditions so applicability to a larger scale is difficult to justify. A-site elements maintain the structure of a perovskite and act as a support for the B-site cations to migrate, so the assumed stability of the structure is derived mainly from the durability of the A-site. This does not consider the interactions between all the elements within the composition since the majority of the perovskites we analyse are complex which can lead to less stable structures and lower lifetime.
	Lifetime scoring method is based on arbitrarily selected 10 year assessment period.	It was simpler to consider replacements or degradation of performance within decades instead of other time periods. For the PV cell configurations, this did not distinguish between the options as most were found to have a lifetime longer than 20+ years.
	GHG emissions scored for anodic catalysts are assumed from synthesis route however all compositions can be made from the lowest GHG emission synthesis route.	Due to the novelty of the catalysts, this information is not reported on, so some basis had to be found. Since these materials are made by the WP2 teams, synthesis routes were known and could be used for distinguishing the scores. This negatively impacts compositions which were made from higher GHG emission synthesis routes as this is more dependent on the choice of synthesis made by the lab user and does not inherently reflect the composition.
	PM and hydrological toxicity definitions intrinsically disadvantages materials or configurations using a larger range of metals.	This was done to simplify the scoring process and ensure even applicability to the electrolyser considerations as well as with the PV cells. This leads to lower scores for options involving more materials. As an amendment for the final draft, this will

		be considered as a percentage of the materials involved instead of count.
	PM and hydrological toxicity measurements have been extrapolated from UK reports despite locations of REFINE plants are not defined yet.	This assumption was made to make a more comprehensive scoring process for these two criterions, so this location was selected as the reports were easily accessible to the researcher. This does not accurately reflect the situation in other potential REFINE sites so this can be omitted from consideration when scoring within the final draft.
	Recyclability scores for PV cells were assumed more from qualitative reports. This also does not follow the definition of recyclability attached to the methodology since these are full configurations instead of individual materials.	To find the number of cycles of recyclability in each of the materials involved in each PV cells configuration would be time consuming and difficult. Additionally, applying this logic to the scoring assumes the recyclability of the separated pure material. The scoring for each option may be more open to dispute as there could be author biases from the literature used to describe the recyclability of the configurations.
	Some scores for the anodic substrate do not follow the criteria definitions listed in the methodology and instead more of a comparative analysis was employed. i.e. Lifetime scored Ti mesh higher due to this material generally being stronger than Ni.	Since there are less alternatives considered for this electrolyser component, these assumptions were made to ensure more distinguishability between the two options. This complicates the justification of the scores as readers are unable to attribute these to the described meanings and must rely on the discretion of the author.
Economic	Capital costs associated with the electrolyser component have been calculated from pure metal market prices instead of precursor versions.	Again, due to the novelty of some of the compositions used and limited reporting on this criterion, estimations had to be made. The metals comprise the bulk of the cost of each of the compositions so to ensure impartiality between each option, prices of the pure metal were calculated from the composition. For each composition, the metals would have been extracted from much cheaper precursor carriers, so this does not accurately reflect the material cost as some compositions may be cheaper to manufacture depending on their precursor.

Capital costs calculated from electrolyser components do not consider operational or logistical costs i.e. labour, heat, transport etc.	At this stage of WP14, these considerations are difficult to estimate so have been omitted to avoid incorrect calculation. This simplifies the definition and does not capture the full significance of this criterion. However, over the course of the REFINE timeline, the costs of these materials can potentially be more accurately estimated from TEA.
Metal market prices are dynamic and change daily so some prices may have changed since calculation.	There is limited significance in the difference in prices of the materials when compared to a few months ago so it can be assumed that the price estimations will be relatively similar to when they were first calculated. Significant changes may lead to inaccuracies to the scores meaning a material could be more economically viable than another.
Capital cost scores found for PV cell configurations have referenced a range of data types and resources from price per unit power produced, descriptive comparisons, readiness and accessibility of technology i.e. newer technologies are inherently more expensive.	Due to lack of reporting for comparable cost types for the technologies, this was found to be a faster solution in contrast to the continual search for similar values. The scores can be disputed as they are derived from a diverse set of data types and units which presents a disproportionate representation for each of the cell configurations.
Maintenance costs have not been considered apart from cost of replacements.	Maintenance information was not found to be widely reported so this was omitted to avoid inaccurate estimations. Scores can potentially be higher than estimated as some options may only require cheaper maintenance treatments rather than complete replacement.
Replacement cost scores use an arbitrarily selected 10 year time period.	As with the Lifetime criterion, this time period was used to simplify calculation as the scores for this were derived from this criterion. This may visualise an incomplete lifecycle for some of the options which have a lifetime longer than 10 years. Additionally, this misleads comparisons as this does not distinguish between material options

		which require replacement more than this time period e.g. a material which requires replacement every 11 years is scored equal to that of a material which can last 20+ years.
	Replacement costs use an average score extrapolated from the scores given for capital cost and lifetime.	This was performed to simplify the scores made for this criterion as information on future changes to costs would be difficult to consider at this stage of WP14. This assumption disregards cost changes attributed to the advancement of these technologies i.e. options may require less frequent replacement or may be more affordable due to market demands.
	Disposal/treatment costs are assumed from the waste hazard classification reported by the UK government.	These reports were most accessible to the author, and it is assumed that this will have close likeness to waste classifications from EU countries. Significant differences to other nations' waste hazard classifications can lead to alternative scores however once REFINE locations have been decided, these scores can be adjusted.
	Disposal/treatment costs are scored qualitatively i.e. based on hazardous content requiring more specialised treatment hence elevated costs.	Specific costs associated with the disposal or treatment of the options were difficult to find so an estimate was used from this definition. Non-hazardous materials can still accrue high disposal/treatment costs, and this assumption generalises potential fees from complex handling procedures. Alternatively, hazardous materials do not necessarily result in high costs as facilities may already be in place to manage these.
Social	Human toxicity scores for the electrolyser also do not consider other substances, solvents or chemicals which can also pose harm to human health.	The assumption to attribute toxicity concerns to only the metals present in the composition is to simplify the analysis as well as to ensure level comparison between all compositions i.e. avoids non-material based toxicity from different synthesis routes/manufacturing processes. This is not a full representation of the hazards associated with the materials lifecycle and those with more dangerous manufacturing procedures

		are generalised with materials which use a safer process.
	Carcinogenicity for the electrolyser assumes only harm from the metals in the final composition instead of other materials used during synthesis/manufacture.	Again, this assumption is used to simplify the analysis as listing all of the substances and chemicals used for each material and finding carcinogenic information is tedious and can be inaccurate since it may not be representative of actual lab work. Likewise, this misrepresents potential carcinogens involved in the synthesis/manufacture of these materials.
	Mining implications only consider a limited group of ethical aspects.	The report used to formulate the scores for this criterion only describes these ethical violations, so this was maintained to simplify the analysis. Again, this may misrepresent some materials/configurations where other violations may apply.

3 MCDA Electrolyser: Considerations

Applying the MCDA methodology to material considerations with the electrolyser revolved around the electrode components to support the work being conducted by WP2 and WP5 members. The options were provided by these teams and these represented materials for the catalyst and substrates for the anode and cathode.

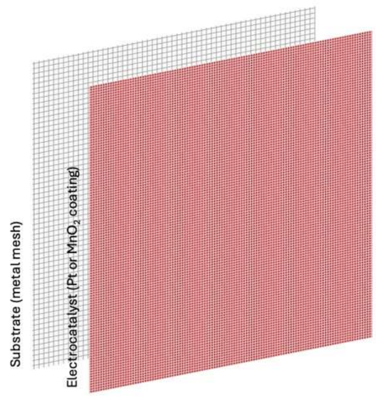

Figure 4: Diagram of Cathode Layers

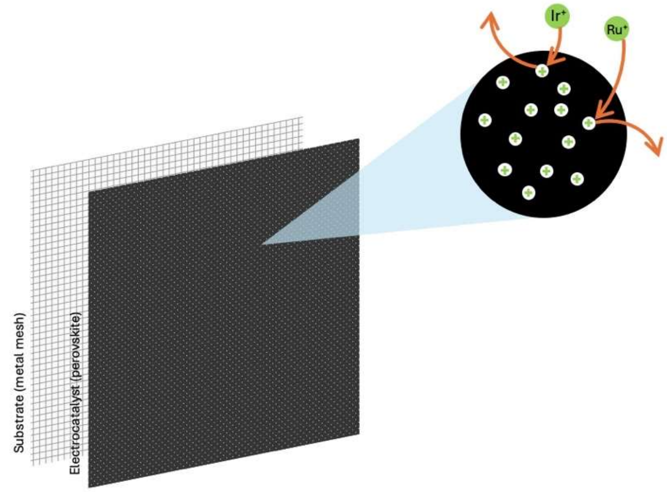

Figure 3: Diagram of Anode Layers with Schematic of Galvanic Replacement Process

The decision for the materials used in the design of these components is paramount for ensuring fast kinetics and improved efficiency with the entire electrolytic system. From Figures 3 and 4, it can be observed that the substrate serves as a carrier for the catalyst to provide structural support as well as facilitate with electron transfer. The catalyst, however, provides the active sites to accelerate the electrochemical reactions which occur at the electrode surface. Therefore, it is justified that the application of MCDA is required here to consider non-technical parameters which can provide alternative recommendations to work package teams assessing these materials experimentally.

For the anode, the substrate and catalyst are considered separately due to the novelty with some of the materials considered for the latter. Substrate options have been advised as **Titanium mesh and Nickel mesh** which are more common materials for this purpose. In the analysis of catalysts, these proved to be more diverse, but options remained with perovskite oxide structures with the general formula of ABO_3 due to their inherent electric and catalytic activities as well as established ability to combat high overpotentials caused by the Oxygen Evolution Reaction (OER). We analyse ten perovskite structures including:

- **STF** (Sr, Ti, Fe)
- **STFC** (Sr, Ti, Fe, Cu)
- **STFN** (Sr, Ti, Fe, Ni)
- **LSTN** (La, Sr, Ti, Ni)
- **BSCF** (Ba, Sr, Co, Fe)
- **BSCFN** (Ba, Sr, Co, Fe, Ni)
- **BGLC** (Ba, Gd, La, Co)
- **BGLCF** (Ba, Gd, La, Co, Fe)
- **BGLFN** (Ba, Gd, La, Fe, Ni)
- **BGLCFN** (Ba, Gd, La, Co, Fe, Ni)

Although not currently covered in this report, these materials will be further doped with Ir and Ru ions via galvanic replacement since these are the primary materials used in commercial electrolytic devices due to their enhanced OER activity and stability. In the final draft of this report, more considerations will be applied to these materials since they will have vast impact to economic and environmental considerations due to their elevated cost and rarity. However, this is not currently examined here due to limited understanding of the final compositions that can be successfully achieved from the loading process.

Concerning the cathode, there are fewer options being considered with most of these commonly observed in literature and practice. The novelty with these materials lie within their construction but due to more commonly examined materials the full electrode system can be analysed together. The substrate options are the same with what is considered with the anode. However, the catalysts options are split between Pt and MnO_2 where the electrode compositions being analysed are listed as:

- Pt/Ti mesh
- Pt/Ni Mesh
- MnO_2/Ti Mesh
- MnO_2/Ni Mesh

3.1 Matrix, Scoring and Results

Ranked Top in Category:

INDICATOR KEY: ● Technical ● Environmental ● Economic ● Social

Option — Overall Recommendation

	Technical					Environmental				
	BET Surface Area	Particle Diameter	Electrical Conductivity	Overpotential	Tafel Slope	Lifetime	GHG Emissions	PM Toxicity [3], [4]	Hydrological Toxicity [5]	Recyclability
STF	2	2	2	2	4	2	4	4	1	3
STFC	3	3	3	3	3	2	2	2	0	3
STFN	2	4	4	2	1	2	2	2	0	3
LSTN	2	2	4	2	1	4	2	4	1	3
BSCF	2	1	4	4	2	2	2	2	1	3
● BSCFN	3	2	5	4	4	2	1	1	0	3
● BGLC	2	2	3	2	2	4	2	4	4	3
BGLCF	3	3	3	2	4	4	1	2	2	3
BGLFN	3	3	3	3	3	4	1	2	2	3
BGLCFN	3	3	3	2	4	4	1	1	1	3

Anode Catalyst

Anode Catalyst

	Economic			Social		
	Manufacture/ Procurement [6], [7]	Replacement	Disposal [8]	Toxicity to Humans [9]	Carcinogen [10]	Mining Impacts [11]
STF	5	4	5	4	4	5
STFC	5	4	4	3	4	4
STFN	5	4	4	3	1	4
LSTN	5	5	4	4	1	2
BSCF	4	2	5	3	2	4
BSCFN	3	3	4	2	0	2
BGLC	4	4	5	4	3	2
BGLCF	4	4	5	3	2	2
BGLFN	3	3	4	3	1	2
BGLCFN	4	4	4	4	1	0

Cathode Catalyst	Technical: BET Surface Area	Technical: Particle Diameter	Technical: Electrical Conductivity	Technical: Overpotential	Technical: Tafel Slope	Environmental: Lifetime	Environmental: GHG Emissions	Environmental: PM Toxicity [3], [4]	Environmental: Hydrological Toxicity [5]	Environmental: Recyclability
Pt/Ti Mesh	3	4	3	4	5	5	2	5	4	5
Pt/Ni Mesh	4	4	3	5	4	4	4	4	4	5
MnO2/Ti Mesh	3	2	3	3	1	5	2	4	2	5
MnO2/Ni Mesh	3	1	3	2	1	4	4	2	2	5

Cathode Catalyst	Economic: Manufacture/ Procurement [6], [7]	Economic: Replacement	Economic: Disposal [8]	Social: Toxicity to Humans [9]	Social: Carcinogen [10]	Social: Mining Impacts [11]
Pt/Ti Mesh	2	2	4	4	5	4
Pt/Ni Mesh	2	2	4	2	1	2
MnO2/Ti Mesh	5	5	4	4	5	4
MnO2/Ni Mesh	5	4	4	2	1	2

Anode Substrate	Technical			Environmental				
	Electrical Conductivity	Corrosion Resistance	BET Surface Area	Lifetime	GHG Emissions	PM Toxicity [3], [4]	Hydrological Toxicity [5]	Recyclability
Ti Mesh	4	5	4	5	4	5	4	5
Ni Mesh	5	4	4	4	5	4	4	5

Anode Substrate	Economic			Social		
	Manufacture/ Procurement [6], [7]	Replacement	Disposal [8]	Toxicity to Humans [9]	Carcinogen [10]	Mining Impacts [11]
Ti Mesh	5	5	5	5	5	4
Ni Mesh	5	4	5	4	1	4

3.2 Discussion of Domains

From the matrices we can list the primary recommendations for the anode as STF on Ti mesh and for the cathode as Pt on Ti mesh (Pt/Ti) as these have attained the highest overall score across the domains and criteria. However, the tables also indicate the materials which perform optimally in each of the explored categories so we can further evaluate how this may influence the overall selection if alternative weightings had been applied.

Technical

The scoring metrics applied to the technical parameters are more general than those assigned to the environmental, economic and social domains as the criteria used, tend to be more quantitative in nature. The following tables indicate data found from literature and assists in justifying the scores given. Where there is an ‘x’, this indicates information that was unreported.

Table 12: Data Found in Literature for Catalyst Options

Material	BET Surface Area	Particle Diameter	Electrical Conductivity	Overpotential	Tafel Slope
STF	2.63 [12]	0.154 [12]	1.8-2.25 [12], [13]	441 [14]	63.8 [14]
STFC	x	x	x	x	x
STFN	4.55 [15]	0.02-0.07 [16]	23.9 [15]	412 [17]	103 [17]
LSTN	2.1 [18]	0.3-0.6 [19]	22 [20]	495 [21]	106 [18]
BSCF	2.4 [22]	1-10 [22]	16.5 [23]	260 [24]	94 [24]
BSCFN	x	0.5 [25]	40.5 [26]	278 [27]	47.98 [27]
BGLC	4.79 [28]	0.42 [28]	x	500 [29]	85 [29]
BGLCF	x	x	x	410-490 [29]	68-76 [29]
BGLFN	x	x	x	x	x
BGLCFN	x	x	x	451 [29]	61 [29]
Pt/Ti Mesh	x	0.0074 [30]	x	305.9 [31]	30 [32]
Pt/Ni Mesh	1.273 [33]	0.0031 [33]	x	100 [33]	72 [33]
MnO2/Ti Mesh	x	x	x	x	190 [34]
MnO2/Ni Mesh	x	5-8 [35]	x	508 [36]	107 [36]

Table 13: Data Found in Literature for Substrate Options

Material	Electrical Conductivity	Corrosion Resistance*	BET Surface Area
Ti Mesh	$2.5*10^4$	-1.53	x
Ni Mesh	$1.4*10^5$	-0.23	x

*The corrosion resistance was found from corrosion potential values where more negative values are found to be more likely to corrode.

Environmental
BGLC on Ti mesh is found to be most ideal when prioritising environmental factors. From the matrix tables, we see that the catalyst averages a score of 3.4 in this domain, performing best in lifetime, PM toxicity and hydrological toxicity. The literature finds that this material contains only one contaminant currently monitored in the UK posing as a concern for PM and hydrological toxicity. Double perovskites are generalised to have better stability than single structures and the addition of La is found to provide additional stability which supports the top score awarded for lifetime.

Pt on Ti mesh and Ni mesh scores highest in this category with an average score of 4.2. The top-performed criteria between these options include lifetime, PM toxicity and recyclability. For Pt/Ti, the Ti mesh was primarily considered during the scoring for stability since this comprises a larger proportion of the component and this was found to be more durable than the Ni mesh. This was also found to contain no currently monitored contaminants hence the top score. Again, the substrate was prioritised for the recyclability criteria and since both metals are 100% recyclable, these options were awarded top scores.

Economic
STF on Ti mesh scored optimally in the economic category with top scores across all the criteria for the substrate and manufacture/procurement and disposal cost for the catalyst. Ti is found to be more durable than Ni, so this has been awarded a top score in the replacement category as lifetime has been assumed to be longer. Again, since Ti is widely recycled this was scored highly as disposal/treatment costs are expected to be low and market prices of Ti were found to be lower than that of Ni as well. STF uses very affordable metals with the calculated metal price found to be €10.87/kg and disposal costs were assumed to be minimal due to containing no hazardous materials.

MnO_2 on Ti mesh was found to score highest in this category with top scores in manufacture/procurement and replacements. Manganese is significantly more affordable than Platinum with a market price of €2.20/kg and due to the durability of Titanium, replacement costs were assumed to be low as well.

Social
STF on Ti mesh again performed optimally across the social domain scoring top in the carcinogen criterion for both catalyst and substrate and also top in mining impacts for the

catalyst. Both of these materials were found to not contain any carcinogens and STF was further found to lack any metals associated with ethical violations.

Two options were found to perform best in this category: Pt/Ti and MnO_2/Ti which match in scoring across the criteria. Both of these do not contain any carcinogens and only one metal found to be toxic to human health. Additionally, these materials contain at least one material found to have two ethical violations associated with their mining which is relatively low to other materials.

4 MCDA PV Cell: Considerations

The structure of a PV module contains seven layers: frame, glass, front and back encapsulants, PV cell, back sheet and junction. The application of the methodology for the PV module diverges from the electrolyser as this is used to evaluate complete technologies instead of individual materials and components. This approach aligns with the strategies of the PV technical team in sourcing commercial options.

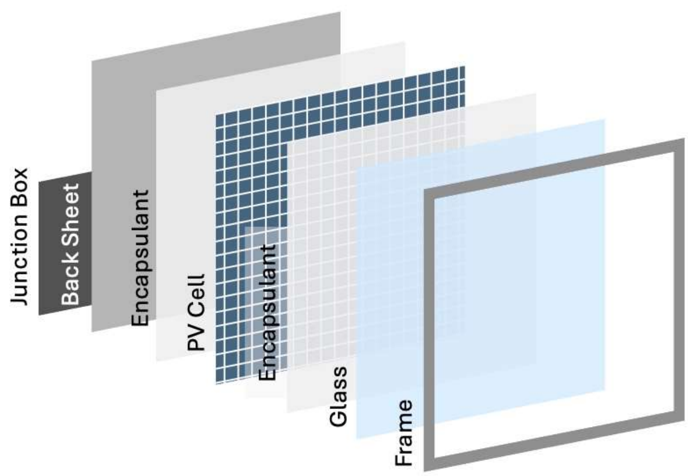

Figure 5: PV Module Configuration

The structure of a PV module comprises of seven layers: frame, glass, front and back encapsulants, PV cell, back sheet and junction box in the order presented in Figure 5. The methodology focuses on the PV cell layer as this controls the solar-to-electrical energy conversion and determines the performance of the module in conversion efficiency as well as stability over time and against environmental stresses i.e. temperature fluctuations, weather exposure etc.

As advised by the WP6 team, five PV cell configurations were examined of the monocrystalline structure as these boast reliably high efficiencies. From this cell category, the following technologies have been examined:

- **IBC** – Interdigitated Back Contact
- **HJT/SHJ** – Heterojunction/Silicon Heterojunction
- **TOPCon** – Tunnel Oxide Passivated Contact
- **MonoPERC** – Mono Passivated Emitter & Rear Cell

- **Perovskite/Silicon Tandem**

These technologies represent varying degrees of commercial maturity, with MonoPERC and IBC options having well-established positions in the industry. This is followed by HJT/SHJ and TOPCon which are relatively recent commercially available options. The Perovskite/Si Tandem cell is an emerging technology, with performance metrics currently limited to laboratory scale testing so far.

4.1 Matrix, Scoring and Results

Ranked Top in Category:

INDICATOR ● Technical ● Environmental ● Economic ● Social | Option | Overall Top Scorer

	Technical					Environmental				
	Energy Consumption	**Thickness**	**PCE**	**Stability**	**Temperature Coefficient**	**Lifetime**	**GHG Emissions**	**PM Toxicity [3], [4]**	**Hydrological Toxicity [5]**	**Recyclability**
IBC	4	4	4	2	2	5	4	1	2	3
HJT/SHJ	4	2	4	2	4	5	4	2	2	3
● **TOPCon**	2	4	4	4	4	5	2	1	2	3
MonoPERC	2	2	2	2	2	5	2	1	2	3
Perovskite/Si	3	3	5	1	4	1	3	0	0	3

	Economic			Social		
	Manufacture/ Procurement [37]	**Replacements**	**Disposal [8]**	**Toxicity to Humans [9]**	**Carcinogenicity [10]**	**Mining Impacts [11]**
IBC	2	2	4	1	1	0
● **HJT/SHJ**	2	2	4	1	1	1
● **TOPCon**	4	4	4	1	1	0
● **MonoPERC**	4	4	4	1	1	0
Perovskite/Si	1	1	3	0	0	0

4.2 Discussion of Domains

Technical

Similarly to the electrolyser section, data found from literature is presented with the technical domain due to the simplified scoring metrics. Table 14 compiles a range of quantitative and qualitative data to assign the scores.

Table 14: Data found in Literature for PV Technology Option

PV Cell	Energy Consumption	Thickness	PCE	Stability	Temperature Coefficient
IBC	Mature manufacturing process	150 [38]	21-24.4 [39], [40], [41], [42]	UV light and temperature Instability [43]	0.35 [44]
HJT/SHJ	Low temp, short process	180 [45]	25.2-26.7 [46], [47], [48]	UV light instability [49]	0.26 [44]
TOPCon	Longer complex process, high temperature	160 [50]	23.91-26.0 [51], [52]	Good thermal stability [53]	0.29 [54]
MonoPERC	Long complex process, high temperature	150-170 [55]	23.5-24.0 [46], [52]	UV light and temperature Instability [49]	0.37 [44]
Perovskite/Si	x	x	27.3-28.0 [56], [57], [58]	Challenges with structure, material processing and general stability [49]	0.26 [58], [59]

Environmental

SHJ scored top in this category, performing best in lifetime and GHG emissions. Due to the scoring metrics applied in the methodology, most of the other technologies scored well in this criterion due to average lifetimes lasting around 25 years. Despite a lack of quantitative data supporting the GHG emission score, this was awarded highly due to the manufacturing process involving less steps and lower temperatures in comparison with the manufacture of other PV technologies.

Economic

TOPCon and MonoPERC are found to perform optimally in this category with matching top scores across the criteria. Despite the relative commercial newness of TOPCon, these have been described to have a good balance of efficiency and stability associated with their cost in comparison to other options in the market. Likewise, with MonoPERC, despite long and complex manufacturing processes, due to their popularity, these have become affordable options for their performance.

Social

Unlike the electrolyser MCDA which analyses materials for each design component, we are considering full devices for the PV module which potentially contributes to the poor scores across all the criteria within this domain. The top scoring cell configuration is SHJ however this only achieves an average score of 1. This option contains three heavy metals monitored for toxicity to humans and contains one group 1 carcinogen which is with the production of Aluminium for Aluminium-doped Zinc oxide (AZO) rear contacts.

5 Summary of Findings and Recommendation

This study conducted a comprehensive material selection analysis to determine optimal design choices for the components involved in the construction of Unit 1. In alignment with the objectives, recommendations were developed through a holistic approach combining sustainability metrics alongside traditional performance indicators. This methodology is not only in fulfilment with the purposes of WP14 in bridges these concerns but establishes a preliminary framework to support the technical teams in comparative analyses.

The scope identifies three design elements in the electrolyser which required the application of this methodology: anode catalyst, anode substrate and cathode catalyst/substrate. We evaluate ten perovskite compositions for the anode catalyst; two metal meshes with the anode substrate, and four configurations with the cathode. Additionally, analysis of the PV module comprised of five configurations of PV cells. Through evaluation of technical, environmental, economic and social criteria, we were able to conduct our assessment to find the following primary recommendations:

- Anode catalyst: STF
- Anode substrate: Ti mesh
- Cathode: Pt/Ti mesh
- PV cell: TOPCon

The study employed an MCDA, supported by extensive literature review to enable the identification of both primary and secondary recommendations. The procedure also allowed for the recognition of optimal candidates within the assessed domains, permitting an alternative recommendation based on personal requirement or interests.

While the methodology incorporated detailed criteria definitions and scoring metrics, this also highlights the assumptions made during the course of the study. Many of these assumptions can be attributed to the novelty of the materials assessed, however, some of these are due to gaps in literature. Compiling the most significant assumptions leads us to the following list:

- Weighting development was limited to WP14 team input
- Scores determination was primarily conducted by the author
- Non-technical parameter development was again restricted to the discussions of the WP14 team

These assumptions introduce potential limitations, particularly regarding the accuracy of weightings and scores, which may affect the identification of optimal candidates. To tackle these limitations, the final methodology will incorporate the Delphi technique, enabling greater consultation with the technical teams for collective decision-making on critical assumptions. Overall, despite some methodological oversights, the study successfully achieves its primary aim in identifying evidence-based material recommendations.

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