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Sustainable design of multiscale CO_2 electrochemical conversion

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Abstract

The storage of renewable electricity in chemical bonds is a compelling technological option that combines flexibility with the synthesis of high energy-dense fuels and chemicals and may use CO_2 as raw material. The electrochemical conversion of CO_2 is not yet a mature technology. Both fields, electrochemical conversion and carbon dioxide utilisation (CDU), have their own trade-offs; CO_2 electrochemical reduction (CO_2ER) environmental and economic performance is highly context-dependent. The successful deployment of CO_2 electrochemical conversion will depend not only on the further development and scaling of the technology but also on finding appropriate combinations of technologies, business models, and socioeconomic strategies.

The current project aims to create critical knowledge on the sustainable implementation of CO_2 electrochemical devices for a variety of contexts. The research approach presented in the current work will develop a multidisciplinary framework to assess the contributions and trade-offs of CO_2 electrochemical systems, including centralised and decentralised configurations, which are evaluated under realistic conditions. This is a crucial step in understanding the role and contribution of CO_2ER within the different CO_2 mitigation options in place in the upcoming years.

To achieve the project's goal, we propose a multidisciplinary methodology that includes process systems engineering (PSE) and operations research (OR) tools, and humanistic and social sciences methodologies. Modelling and optimisation techniques, value-sensitive design, and identification of government and market-based governance interventions will help identifying potential areas of improvement and bottlenecks to successfully bring CO_2ER to the market. The assessment will be performed at several levels: unit (reaction pathways), process (scheduling and operation, plant layout optimisation), supply chain (optimisation under deterministic and stochastic conditions), and system (social, governance and markets perspectives) of CO_2ER.

The project results will (i) propose optimal CO_2ER-based plants and (ii) supply chains under different contexts; (iii) translate stakeholders' sustainability value into design requirements for CO_2ER; (iv) propose a list of government interventions and market mechanisms that will allow CO_2ER market penetration, and (v) identify, quantify and mitigate the influence of the most relevant sources of uncertainty.

Keywords: CO_2 electrochemical reduction; CO_2 utilisation; multiscale modelling; sustainable design.

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1. Introduction

With a growing trend of global energy demand and increasing attention to the need for climate change mitigation, actions must be taken to switch from a traditional fossil fuel-based to a mainly renewable-based society. Global challenges are also welfare and equity. In transitioning towards a renewable-based society, promising emerging technologies must support variable renewable electricity generation and use alternative carbon sources. However, most of these promising technologies are in their infancy, and implementation conditions may remain unknown during the early stages of development. To be successfully implemented at a commercial scale, emerging technologies must prove sustainable from a social, environmental, and economic perspective.

Carbon dioxide electrochemical reduction (CO_2ER) converts CO_2 and water into fuels, chemicals, or materials using electricity as the main utility (or feedstock). The potential of such technology depends on the availability of renewable electricity and the needs of the renewable plant, as the consumption of electricity to convert CO_2 and water is usually larger than the electricity consumption of the (conventional) fossil fuel-based synthesis processes. The environmental benefit of CO_2ER vs alternative processes should be carefully assessed, and its potential economic performance must also be well understood [1,2]. This project (as described in the current paper, which includes the methodology and aimed results of the two Dutch-funded projects, “Addressing the multiscale challenge of CO_2 electrochemical reduction” and “Sustainable design of multiscale CO_2 electrochemical conversion”, concluding in 2025) aims to contribute to the state-of-the-art knowledge on these aspects by elucidating and evaluating CO_2ER process and supply chain configurations, business models, and socioeconomic strategies.

Nomenclature

CDU	Carbon dioxide utilisation
CO_2ER	Carbon dioxide electrochemical reduction
KPI	Key performance indicator
OR	Operations research
PSE	Process system engineering
SC	Supply chain
TEA	Techno-economic assessment
TRL	Technology readiness level

2. CO_2 utilisation and electrochemical conversion

Carbon dioxide utilisation (CDU) refers to the use of (captured) CO_2 to synthesise products, enabling the utilisation of CO_2 as raw material. This transformation requires significant amounts of energy due to the high thermodynamic stability of the CO_2 molecule. Thermochemical, electrochemical, and biochemical routes are the three main routes investigated to break the chemical structure of CO_2 via heat, electricity and microorganisms, respectively. In general, CO_2 hydrogenation is still an expensive technology, but it is expected that further societal commitment to environmental goals may make this technological option attractive for implementation.

In the last 5-10 years, research exploring the potential industrial implementation of direct CO_2 conversion via the electrochemical route, CO_2ER, has gained interest. First techno-economic assessments (TEAs) [2–4] have sketched the contours of economic feasibility for CO_2ER. To do this, these TEAs used models based on lab-scale performance indicators to estimate industrial-scale production costs of CO_2ER products. The main focus of these analyses has been to compare the techno-economic performance of different CO_2ER products with each other. The results indicated that CO_2ER could be economically feasible for a variety of C1, C2, and even C3 products (i.e., syngas, olefins, alcohols) [2–5]. More recently, the projected production costs for different CO_2ER products were analysed and compared between nine different TEA studies, showing significant cost differences between them [6]. It has been concluded that the projected CO_2ER production costs are likely to be too optimistic in comparison to the production costs of the conventional processes [6]. The techno-economic potential of CO_2ER at industrial-scale remains uncertain, which may be due to the heterogeneity in methodological assumptions, together with assumed optimistic operating conditions (like continuous mode of operation, current or lower-than-current prices, and costs) [6]. In the same context, the environmental impact of such a technological option is also uncertain and hardly explored.

The operating mode is a key design decision and it is directly related to the process economics [7]. Renewable energy sources (i.e., wind and solar) are intermittent by nature. Electrolysers have the potential of handling fluctuating electricity inputs (i.e., flexibility at equipment level [8][9]). The fluctuating electricity will also lead to fluctuations in the product quantities (i.e., volume flexibility [8][9]). Furthermore, based on experimental studies and white-box models, it is expected that the fluctuating electricity supply will also affect the product qualities (i.e., product flexibility [8][9]). Moreover, the connection with a renewable electricity source may influence the CO_2ER-based plant's electricity consumption via electricity price fluctuations [10]. It can thus be concluded that the plant's operation mode, layout, and scale are crucial to determining the optimal techno-economic and environmental performances, not only of the plant itself but also of the overall supply chain (SC).

3. The size of the CO_2ER unit

As mentioned in the previous section, a crucial variable in CO_2ER-based plants and SCs is the adequate (optimum) implementation size of the unit. Currently, CO_2ER is at low technology readiness level (TRL) and there is still significant uncertainty towards industrial scale implementation. The size of a plant may respond to reactor, feedstock, utility or market needs. Three main type of stakeholders were identified that can have a role into the size and speed of CO_2ER implementation,

- the renewable energy plant (with a variety of daily and seasonal patterns) as an electricity provider,
- the chemical industry (with well-stablished capital-intensive fossil fuel conversion processes), that aims at its decarbonisation via electrification and,
- the source of CO_2, e.g. an energy intensive industrial plant (with flue gases at various CO_2 concentrations), that needs to decrease its unavoidable CO_2 emissions (i.e. linked to raw materials conversion).

The electrochemical conversion of CO_2 entails the use of water as feedstock. Moreover, critical materials may be used to fabricate the electrolyser or any of other plant units. Therefore, the size of the plant may be also influenced by,

- the amount of water consumed and,
- the availability of a specific critical material.

The chemical manufacturing industry has historically been developed using economies of unit scale to reduce the capital and operating costs; this includes all possible benefits associated with increasing the total output, building and operating larger individual units. The economies of unit number, contrary to the traditional model, promotes the benefit of facility-level mass production, modular, small unit scale technology and improvements to process design resulting from repetition (a learning-by-doing approach) to reduce the capital costs. This has been at the basis of renewable energy development. The smaller scale reduces cost and time for commercial facilities, enabling rapid and widespread deployment [11].

There are intrinsic adaptability and diversification benefits that can only be achieved via small-scale units; for instance, smaller plants can be installed in multiples to better match a specific output requirement (i.e. selectively run a variable number of the small units), can be installed sequentially as a certain demand evolves, can be installed earlier as a higher technological readiness level is being achieved for a smaller implementation scale, and the required investment cycle can be shorter, as less capital expenditure should be required upfront, not only for the plant itself but also for the required infrastructure [11]. Examples of decentralised hydrogen generation and bio-based conversion processes point out the economic advantage of transporting hydrogen and biomass for shorter distances [12,13].

In the CO_2ER-based plant layout, reactors and gas separation units benefit from a certain level of centralisation through economies of unit scale, and electrochemical reactors, membranes and heat exchangers ("area-based") benefit from economies of unit number. Regarding the CO_2ER-based SC, smaller scale units offer the locational option of centralisation and decentralisation.

An optimum CO_2ER plant implementation size range is still unknown. The size of the plant may respond to the reactor, feedstock, utility, or market needs; however, the final decision should be made concerning the system as a whole and not only to the electrochemical reactor or to any input/output variable alone. The overall objective of the current project is to understand under which conditions CO_2ER becomes feasible for implementation. There are three main sub-objectives:

1. Elucidate the most relevant CO_2ER implementation scales and operating conditions, in different selected contexts,
2. identify business cases according to sustainability indicators, and
3. explore the socio-techno-economic-political nexus since the early stages of implementation (i.e. CO_2ER is at low TRL).

This project brings together a multi-disciplinary approach that takes into account the main CO_2ER players/factors/uncertainties, to understand the gap between laboratory research and practice; a combination of process design and optimisation, supply chain optimisation under stochastic and deterministic conditions, participatory studies and the consideration of sustainability' three sides.

4. Sustainable design

Sustainability is defined as the potential for long-term maintenance of well-being, which has economic, environmental and social dimensions [14]. Accordingly, sustainable development aims at simultaneously creating economic prosperity, environmental quality and social equity [15]. A sustainable life cycle perspective not only considers the electrochemical conversion facility, but also the whole product life cycle. The economic and environmental criteria derive into quantitative well-established key performance indicators. In contrast, the social criterion is highly decision-maker dependent and may be captured by both, qualitative and quantitative indicators. Sustainability is an overarching value that comprises other values. In addition, it can be perceived differently by different stakeholders. Sustainability and its associated values can therefore change over time, responding to the occurrence of new moral problems, new social behaviors or emerging public debates [16]. Changes in value can then lead to controversy, and in turn to project failure. Addressing or even avoiding such mismatches requires a better understanding of the central value of sustainability and how it may change over time.

The current project will contribute to filling the gap in the study of the sustainability of CO_2ER by developing realistic case studies in collaboration with stakeholders. The inherent characteristics of CO_2ER expose a multi-stakeholder complex problem (see Fig. 1) with many exogenous and endogenous uncertainties that can compromise the long-term sustainability of the system. It is essential to take those uncertainties proactively into account in decision making in order to make the system design "future-proof" (with the current available knowledge), rather than assuming that current conditions will remain unchanged, or that the future state of the conditions can be estimated with certainty (for instance, assuming current prices or current economic structure). CO_2ER and CDU are neither intrinsically sustainable or unsustainable, and we aim at contributing to understanding (i) if the technology can be acceptable to society and (ii) its potential as one of the solutions of the new energy paradigm. According to Fig. 1, there are many variables in the commercial implementation of CO_2ER, for example;

- In the technological context, CO_2ER efficiency depends on the type of electroyser and the product to be synthesised, and as an emerging technology, research focuses on higher conversion efficiencies through the use of cathode-electrolyte efficient combinations.
- From an economic point of view, the CO_2 price for future projects is not yet known, and may change depending on whether CO_2 is a greenhouse gas emission and/or a raw material.
- In a legal context, the prioritised measures to promote and/or fund emerging technologies and to decrease CO_2 emissions, and how CO_2 emissions are accounted when CDU is involved, are relevant.
- In the social context, CDU public acceptance is still unknown.

Overall, the success or failure of the introduction of CO_2ER depends not only on the technological development and the environmental impact, but also on a large number of contextual (resource availability, geography), legal, economic and political-social factors, which can act as barriers or enablers for CO_2ER implementation.

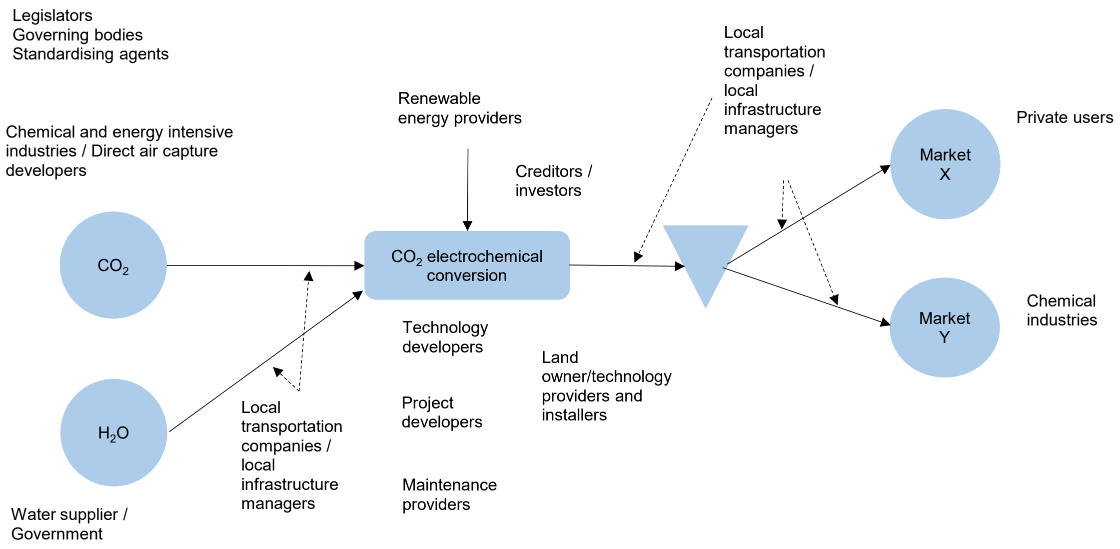

Fig. 1. Simplified map of the many stakeholders that are involved in the CO_2ER (and CDU) supply chain and implementation.

5. Multiscale CO_2 electrochemical conversion

The overall scale levels studied in the project include unit (nano), process (micro), supply chain (meso) and system (macro) scales. In Fig.2, the scale levels are depicted and the bidirectional influence among the process and SC levels with the society plane highlights the embedding of CO_2ER systems in society in the current conceptual design (and ex-ante evaluation) approach.

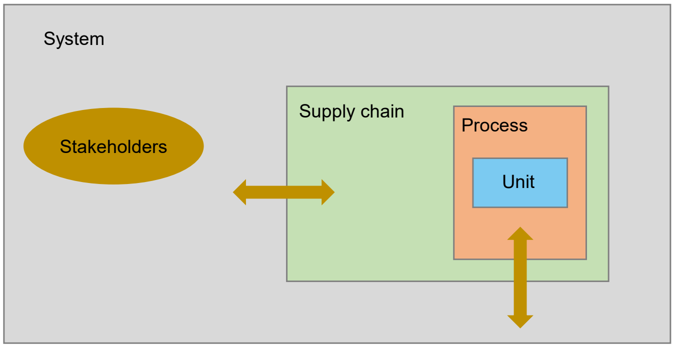

Fig. 2. Representation of the scale levels studied in the project.

5.1. Unit

In this level, we will develop first-principles models for representing a low-temperature and a high-temperature electrolyser. Electrolysers are modular by nature, and the plant size would depend on the market under which it will compete; stacks can be proposed at “any size”, depending on the technology-developers criteria. The aim of the current step is to provide a model detailed enough to avoid misconceptions arising from extrapolating experimental data at laboratory scale and/or operation regimes outside the model calibration conditions, and to avoid errors in process modelling, by explicitly considering the electrochemical principles. The electrolyser configuration will impact the upstream and downstream units considered at process level. To our knowledge, there are no studies publicly available comparing different electrolyser types at a process design level.

The starting point of the electrolysis cells is the work developed in [17], which is a solid oxide fuel cell first principles model, validated for Solid Power cells, incorporating fluid dynamics, finite-element stress analysis, and 3D electron imaging. The model is modular, and assemblies the discretised electrode, cell, channel and plates sub-models. The main governing equations are distributed charge transport and transfer for the electrodes, and the Stefan-Maxwell, dusty-gas model with heterogeneous reactions for the electrode-electrolyte reactions.

5.2. Process

Regarding the industrial implementation of CO_2ER from the process or plant perspective, other aspects that are relevant are:

- Raw materials' conditions. For instance, CO_2 is unlikely to be available as a pure stream, and therefore needs to be further purified before entering the electrolyser.
- Water purity. In general, demineralized water is needed for electrolysis.
- The synthesised product. The product from the electrolyser is normally not pure, and further downstream units are needed to reach the required market specifications.

In the current level, we will analyse different plant layouts, with the purpose of providing a better understanding of the design and size limits, via process modelling and optimisation. Process units are, apart from the electrochemical reactor (incorporated from the previous level), mainly separation units for the recovery of the products and of the electrolytes (if needed and possible), and for CO_2 and/or water purification: liquid-liquid, gas-liquid and gas-gas separators (for instance, distillation, stripping, adsorption, absorption or membranes). Balance-of-plant units are mainly pressure changers and heat exchangers. Storage tanks (and possibly batteries) are also important, in this case, to decouple the discontinuous from the continuous mode of operation of the different plant sections, and to store the final product before market distribution.

5.3. Supply chain

At SC level, size and location of CO_2ER plants and its related transportation network (connection among the SC actors) are unknown. In the CO_2ER SC, the electrolyser-based plant is connected to a renewable electricity provider, a water or hydrogen provider, and to a CO_2 producer on the input side. On the output side, the electrolyser-based plant is connected to a product/intermediate consumer or the chemical industry, and to possible product-storage locations. There is a SC configuration challenge due to different locations and size or scale needs (i.e. for instance, (i) the amount of renewable electricity available can be smaller than the amount of electricity needed, or (ii) the CO_2 supplied by a large-scale point source can be larger than the CO_2 needed as feedstock to fulfill a CO_2ER-based product specific demand).

The optimisation at SC level will incorporate the modelling input from the electrolyser (unit level, reaction pathways) and plant (process level, scheduling and operation, plant layouts), under specific scenarios. The techno-economic and environmental key performance indicators (KPIs) will be evaluated at different time periods, situations, and future development options before and after incorporating social factors, under deterministic and stochastic conditions.

5.4. System

In this overarching level, we will (i) find barriers and enablers of CO_2ER (CDU in general) implementation, (ii) identify economic, environmental and social hotspots of CO_2ER and (iii) address the main sources of uncertainty. Inclusive technology innovation and proactive design are taken into account in the process and SC levels described above (thus this level retrofits the previous two), ensuring that relevant expertise, knowledge and views are incorporated. With this aim, value sensitive design, stakeholders interviews and a systematic analysis of the compiled data are methodological steps which will contribute to the consideration of multiple stakeholders views (not only operational needs, as in the SC level).

6. Perspectives

The project described in the current paper (which includes the methodology and aimed results of the two Dutch-funded projects, "Addressing the multiscale challenge of CO_2 electrochemical reduction" and "Sustainable design of multiscale CO_2 electrochemical conversion", concluding in 2025) aims to contribute to the state-of-the-art knowledge on the techno-economic and environmental performance of CO_2ER, by elucidating and evaluating CO_2ER process and supply chain configurations, business models, and socioeconomic strategies. To this end, the project proposes a multiscale model of the overall CO_2ER-related system, including nano, micro, meso and macro scales models (unit, process, supply chain, and societal models), bringing together a multi-disciplinary approach. It includes PSE and OR tools, and humanistic and social sciences methodologies. The resulting (CO_2 electrolysis-based) modelling platform, will convey the latest and most relevant technology/lab scale knowledge into the ex-ante evaluation and conceptual design of the associated plants and supply chains. It will bridge unit and process scale models, process and supply chain models, while taking into account the social context and stakeholders views.

Acknowledgements

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SUSTAINABLE DESIGN OF MULTISCALE CO_2 ELECTROCHEMICAL CONVERSION

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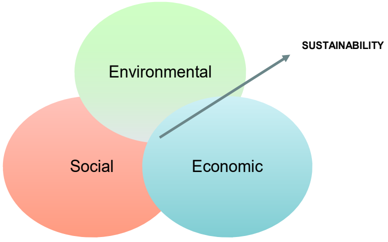
Introduction

- Decreasing carbon emissions in the industry and energy sectors: interest in the electrochemical conversion of CO_2.
- Electrolysers: Modular scale-up with critical specificities at the ex-ante evaluation and conceptual design phases:
  - Plant's size is dependent upon the market under which it will compete.
  - Device design and system integration are dependent upon the objectives of technology developers.
- Challenges in bridging scales:
  - Misconceptions arise from extrapolating experimental data at the laboratory scale and/or operation regimes outside of the calibration conditions.
  - Standard performance/operation metrics are applied without careful consideration of the underlying assumptions, e.g. local/global feed/fuel conversion.

Plant's operation mode, layout, and size range are crucial to determining the optimal operating conditions of the electrolysis-based plant and supply chain. The overall implementation feasibility will be understood by considering the overall system.

Objective: Electrolysis-based modelling platform for conveying the latest and relevant technology/lab-scale knowledge into ex-ante evaluation and conceptual design of associated plant(s) and supply chain(s), and exploring the socio-techno-economic-political nexus.

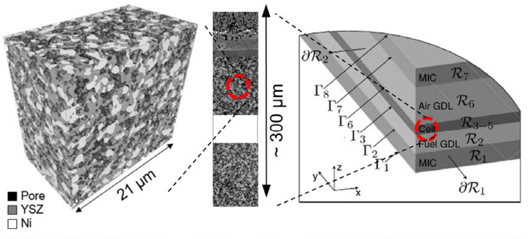
Sustainable design



- Life cycle assessment.
- Collaboration with stakeholders.

1. Cell modelling

- **Approach (solid oxide cell - SOC):**
  - **Modularity:** Assembly of discretised electrode, cell, channel and bipolar plate sub-models.
  - **Level of detail:**
    - "1-D + 1-D" spatial discretisation (large aspect ratio of electrolyzer components).
    - Continuum modelling.
  - **Governing equations:**
    - Composite electrode models with distributed charge transport and transfer.
    - Stefan-Maxwell, Dusty-gas model with heterogeneous reactions.



3-D electron imaging *Cell model* *Layers in fast moduar model*

Collaboration with Dr. Arata Nakajo

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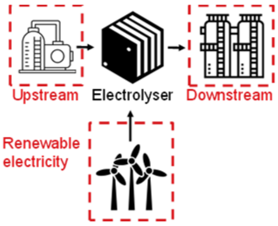
2. Process modelling

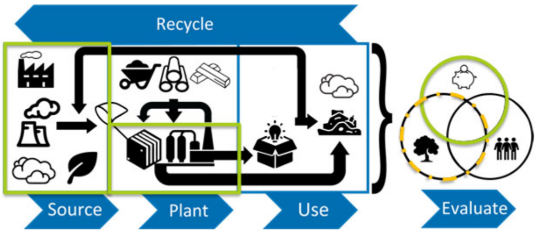
- **Knowledge gaps identified in literature and current work contribution:** *Systematic analysis of techno-economic assessments of electrochemical processes.*



- **Pre-treatment:** Purification of water and CO_2 inlet streams is hardly considered (assumed pure, free, readily available streams).
- **Downstream processing:** Separation and upgrading of the outlet stream is minimally considered (assumed high purity product at minimal cost).
- **Electricity:** The impact of renewable sources' intermittency is not studied (assumed cheap and continuous renewable electricity available).
- Storage strategies are not treated: for instance, tanks for the electrolysis product or batteries.
- Plant optimisation strategies are rarely taken into account: for instance, waste management, recycle effects or heat integration.

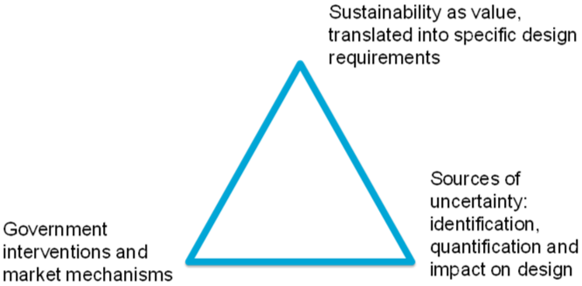
3. Supply chain modelling

- **Knowledge gaps identified in literature and current work contribution:** *Systematic analysis of the effect of feedstocks and technologies on the sustainable design of supply chains for CO_2, hydrogen and biomass.*



- Electrochemical reduction of CO_2 not evaluated from a supply chain perspective.
- Carbon capture and utilisation supply chains minimally described.
- **Modelling approach:** Mathematical modelling (mixed integer linear programming), national supply chains under deterministic conditions, economic drive.
- **Sustainability-based indicators:** Mainly economic indicators. Environmental limited to carbon emissions and social to risk, acceptance or safety.

4. System



Through inclusive technology innovation and proactive design, compilation of relevant expertise, knowledge, and views, the project will:

- Pinpoint the barriers and enablers of CO_2 electrochemical conversion implementation.
- Identify economic, environmental, and social hotspots.
- Address the main sources of uncertainty.

Perspectives

- **Including chemical engineering and operations research tools, and humanistic and social science methodologies, this project will bridge the models at unit and process scales, process and supply chain scales, while taking into account the social context and stakeholders' views.**
  - Extension of the validated operation windows: Direct electrochemical conversion of CO_2.
  - Plant-relevant conditions: Implementation of the effects of stream compositions and conditions (upstream units, downstream units and recycles effects).
  - Quantification of the impacts in the market.

This research receives funding from the project "Addressing the multiscale challenge of CO_2 electrochemical reduction", NWO ECCM tenure track grant (project number ECCM.TT.009) and "Sustainable design of multiscale CO_2 electrochemical conversion", MVI grant (ECCM.TT.MVI.TU.006). Both projects are concluding in 2025.