Light assisted solar fuel production by artificial CO_2 Reduction and water Oxidation

Deliverable D6.3

Environmental, societal and ethical consequences of the LICROX technology

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EXECUTIVE SUMMARY

This document, D6.3 Environmental, societal and ethical consequences of the LICROX technology, is a deliverable of the LICROX Project, which is funded by the European Union’s H2020 Programme under Grant Agreement No. 951843. The deliverable documents the proceedings of T6.1 in WP6 of the H2020 LICROX project. The primary focus of this task has been to map the environmental and societal consequences, barriers and impacts of the LICROX technology. This mapping has been carried out on a basis of two major inputs: (1) A prospective life cycle analysis of the LICROX PEC and (2) stakeholder engagement on the environmental impacts, socioeconomics, and ethics of the LICROX PEC and comparable technologies. The deliverable provides unique insights to the environmental consequences of the LICROX technology and to the societal concerns and barriers that should be addressed at research, societal, or policy level.

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A. Introduction

1. Purpose and structure of this deliverable

This deliverable provides key insights to the environmental impacts and social acceptance of the LICROX technology and constitutes a primary output of WP6 of the LICROX project. The deliverable documents and reflects upon the two major components of T6.1 *Mapping of consequences, barriers & impacts*: First, the prospective life cycle assessment of the LICROX PEC, which provides novel insights to the emerging technology and its environmental impacts. The LCA has been carried out by Dr. Ivan Muñoz from 2.-0 LCA Consultants, subcontracted for the task. Second, the stakeholder engagement, focusing on environmental impacts, socioeconomics and ethics. The framework for the stakeholder engagement is the identification of societal barriers, conflicts, and resistance, which can be applied by the LICROX project to strengthen the technology and its eventual implementation.

The structure of this deliverable follows the chronology of the activities that have been carried out in T6.1: The LCA provides key insights that feed into stakeholder workshops, where the prospective environmental impacts are discussed and contextualized. In this way, one may see the output of the LCA in two stages. First, at its face value, presented as the conclusions of the LCA. Second, as the results of the stakeholder engagement, where environmental impacts influence the societal barriers and recommendations that are identified and laid out in this report. For this reason, the deliverable is structured in three main components: Following section A, where the deliverable is introduced and contextualized, the LCA is presented in section B. This is followed by section C, where societal and ethical consequences are covered and the facilitated stakeholder workshops are documented, leading to a short range of recommendations. In this way, the deliverable presents two conclusions: One for the LCA and one for the stakeholder engagement processes.

The findings of this deliverable feed into T6.2 of the LICROX project *Citizen's perceptions, acceptance, and livelihood – Acceptability assessments.* This task builds onto the mapping of environmental and societal consequences of the LICROX technology to carry out a European-wide investigation of citizen views on emerging energy technologies. The findings also feed into T6.3 *technological resistance, future market potentials and exploitation of LICROX outcomes.* The output of this deliverable naturally covers concerns that affect the eventual implementation of the LICROX technology and its potential marketability. It is thus expected that the environmental and societal concerns, as well as the concluding recommendations are useful for the assessment of a future market potential and the development of an exploitation plan. Last, the findings of the LCA presented in this deliverable should feed into the technological development of the LICROX PEC. The recommendations stemming from the LCA should be understood as research goals, that should be reached for the technology to mature.

2. Contextualizing the need for environmental and societal considerations in emerging energy technologies

With the European Green Deal (European Commission, 2019) the European Commission outlined the urgency for Europe to mitigate and adapt to global rising temperatures and a changing climate. With current projections still pointing toward a catastrophic global temperature increase and greenhouse gas emissions continuously rising, historical efforts are necessary to decarbonize our society. The year 2022 did not only stress our vulnerability to a changing climate, but also our need for a resilient and stable energy system.

Decarbonizing the EU and stabilizing our energy systems are two sides of the same story, as a European phase-out of fossil fuels is the next big step outlined by von der Leyen in the European Green Deal (European Commission, 2019), Fit for 55 (European Parliament, 2021), FuelEU Maritime (EESC, 2021)[1], and REPowerEU (European Commission, 2022). The latter is framed as a response to one of the effects of Russia's military aggression against Ukraine, namely the disruption of the global energy system. A European and global transition is coming, and an increasing number of stakeholders are now working to implement renewable energy sources on European grounds.

Implementation of renewables, like windmills and photovoltaic[2] cells can, however, not cover European needs for energy as is. Renewable energy sources are naturally fluctuating, often producing either too little or too much energy for society to depend on. To stabilize a European energy system, storage of energy becomes the focal point for policymakers and researchers. While batteries and mechanical solutions to energy storage are of use in certain contexts, the current European interest and main obstacles lie in long-term transportable energy solutions. For most purposes, this demand is addressed through Power-to-X (PtX), namely electrolysis and carbon capture and utilization (CCU) technologies, making use of excess energy production and carbon-emitting industry byproducts.

It is generally agreed upon that PtX poses a necessary part of the solution to the energy- and climate crisis (Breyer et al. 2022). However, the energy conversions that PtX facilitates, are intrinsically imperfect, leading to losses of up to over half the energy. For this reason, state-of-the-art energy systems research stresses that the utilization of PtX must be carried out mindfully and only in the sectors where other solutions (like electrification or systemic change) are impossible (Breyer et al., 2022).

The LICROX project approaches the PtX development with a focus on ethylene as an output. LICROX is distinctive in mimicking artificial photosynthesis through the development of a photoelectrochemical cell (PEC), directly converting sunlight, water, and CO_2 into carbon-based molecules (i.e., ethylene). The LICROX technology is expected to be utilized precisely in the sectors where electrification is impossible, namely as fuel for heavy industry processes, fuel for the shipping industry, and/or as feedstock for the (bio)chemical industry. However, as Breyer et al. (2022) highlight, careful thought needs to be put into (1) the technical development of the technology, ensuring that it aligns with societal needs, and (2) the consequences that a grand roll-out of any novel technology will have. This report focuses on the latter, mainly exploring environmental, societal, and ethical consequences of a potential implementation of the LICROX technology.

Because the LICROX technology is still within the emerging field of novel solar fuel technologies, the exercises carried out in this report are prospective and foresight-based. Based on estimations formed from theoretical lab-scale ups, a prospective life cycle assessment (LCA) has been carried out by Dr. Ivan Muñoz from 2.0 LCA Consultants. The LCA identifies and assesses the environmental consequences that are connected to the LICROX PEC, noting that the exercise is carried out on a basis of assumptions derived from the LICROX consortium in addition to relevant literature.

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[1] In addition to renewable fuels, FuelEU Maritime specifies a need for low-carbon fuels.

[2] PV and wind power have grown to dominate the field of renewable energies and are expected to continue doing so. Other prominent forms of renewable energy sources are bioenergy and hydropower, which are still expected to contribute to the future energy system.

B. Environmental consequences

The assessment of environmental consequences of the LICROX technology is approached through a life cycle assessment (LCA), conducted by Dr. Ivan Muñoz from 2.-0 LCA Consultants. The LCA provides an in-depth dissection of the LICROX technology, followed by an assessment of environmental consequences and recommendations for technological improvements. This chapter covers the executive summary of the LCA. The full LCA can be read in annex A.

1. Life cycle assessment

1.1 The LICROX project

LICROX is a Research and Innovation Action project funded by the European Commission under the Horizon 2020 programme. The aim of the project is to produce and test a photoelectrochemical cell (PEC) for converting sunlight into organic molecules. Such organic molecules can then be used either as fuels or as platform chemicals. As part of the LICROX project, a life cycle assessment (LCA) study has been conducted, consisting of two iterations. This report describes the second and final iteration of the LCA study, following the ISO standards on LCA: ISO 14040:2006 and ISO 14044:2006. The study has been subject to a critical review by an independent external LCA expert.

1.2 Goal

The goals of this study are twofold:

- To assess the life-cycle impacts of the LICROX technology at an early stage of development, in order to identify key hotspots and suggest potential improvement options.
- To compare LICROX with a conventional technology to produce ethylene, namely petrochemical steam cracking.

1.3 Systems under study

The target product for the two production processes under study is ethylene, a hydrocarbon with the formula C_2H_4. The most common industrial process for production of ethylene is via steam cracking of crude oil-based feedstocks.

Steam cracking is a petrochemical process in which saturated hydrocarbons are broken down into smaller, often unsaturated, hydrocarbons. Steam cracker units are facilities in which a feedstock such as naphtha is thermally cracked through the use of steam in steam cracking furnaces. The main product from steam crackers is ethylene, but other valuable co-products are produced, such as propylene, C4 hydrocarbons such as butadiene, and pyrolysis gasoline, for example.

Production of ethylene by means of the LICROX concept is assessed considering a hypothetical industrial plant, with an unspecified production capacity, located in Europe. This plant includes the following elements:

- The PEC device, installed in a ground installation, in a similar fashion as in a photovoltaic plant.
- Structural support and piping.
- An ultrapure water production unit.
- A chemical dosing station, from which CO_2 and electrolyte (potassium bicarbonate solution) are supplied.
- Auxiliary devices such as pumps, control and monitoring system, sampling and gas analysis system.

- A downstream processing unit, which will mainly consist of a gas separation process by means of pressure swing adsorption.

The functional unit and reference flow used in the study to compare both systems are 1 kg ethylene. The study can be considered as a ‘cradle-to-gate’ LCA of ethylene, since the downstream stages of ethylene conversion to final products, their use and disposal are excluded. This is justified given that these life cycle stages are expected to be the same regardless of how the ethylene is produced, and therefore they become irrelevant from a comparative point of view.

1.4 Data sources and quality

All activities in the life cycle are ultimately linked in the background to the ecoinvent database, version 3.6, specifically the ‘Substitution, consequential, long-term’ system model.

Production of the PEC device and its underlying components is based on data provided by the consortium on the specific materials incorporated in the device. In many cases, specific inventories have been developed by 2.-0 LCA consultants for a substantial number of materials. These estimated inventories have a high uncertainty. Data on manufacturing the PEC (sputtering, roll-to-roll processing, thermal evaporation, gravure coating, encapsulation) have been compiled by the consortium partner ICFO, to reflect a real industrial process.

Data on the infrastructure needed to build a full-scale LICROX plant were not available. This has been covered with published data describing a solar-assisted photocatalysis plant treating industrial wastewaters in Spain. With these data we attempt to cover the requirements for civil engineering, structural materials, piping, etc. for a hypothetical LICROX plant, excluding downstream processing of the produced gases, the latter included as a pressure swing adsorption (PSA) process, covered by means of literature data on an industrial PSA plant treating biogas.

Data on operation of a hypothetical LICROX plant were equally scarce. A basic mass and energy balance for the overall process has been defined based on reasonable expectations by the consortium, basic stoichiometry, etc. Several key aspects were also suggested by the consortium as a best guess, namely the PEC useful life, the ethylene yield, the carbon dioxide utilization efficiency, the composition and replacement rate for the electrolyte, as well as electricity consumption by the whole plant. Regarding the carbon source, pressurized carbon dioxide from a nearby industrial source is assumed as the default scenario. Finally, the end-of-life stage for the LICROX plant assumes a plausible fate for each material, chiefly recycling/disposal.

Regarding steam cracking, a dedicated model for ethylene production by this technology has been developed. This required, in addition, to develop a model for production of propylene, the main by-product from steam cracking. Both models have been built based on published data on process simulation, providing a sufficiently detailed mass and energy balance for steam cracking using naphtha as feedstock, and for propylene production using methanol as feedstock.

1.5 Impact assessment method

The method used for impact assessment is ‘Stepwise’. In total, this method includes a total of 16 impact categories, which can be expressed in biophysical units (mid-point), and in a common unit expressing damage (endpoint), namely in monetary units.

1.6 Key findings

The main conclusions of the study can be summarized as follows:

- Life cycle impacts from ethylene produced by a hypothetical LICROX production plant, as envisaged in this study, appear to be substantially higher than those for ethylene produced by conventional steam cracking. This is the case for 15 out of the 16 indicators included in Stepwise. As an example, GHG emissions are 34 times higher for LICROX.

- The main driver for environmental impacts of the LICROX technology corresponds to plant operation. Two main aspects are highlighted as key contributors: electrolyte supply and CO_2 supply. The impact of electrolyte supply is closely related to the fact that potassium bicarbonate and ultrapure water need to be added and replaced on a weekly basis, while the impact of Carbon dioxide supply mainly corresponds to the energy use associated to recovering this gas from industrial exhaust gases.
- The environmental impact associated to the PEC as a component of the LICROX plant is not negligible. It can be considered as the second most important aspect after plant operation, and this is closely related to the relatively low ethylene yield. The environmental impact of the PEC is highly dependent on the assumed useful life, which has been taken as 10 years. However, this degree of durability is currently more a hope or a goal than a fact. The main identified contributor to the environmental impact of PEC as a component is the electricity consumed during its manufacturing.
- Other plant infrastructure construction and disposal (including the downstream processing unit) appear to also be relevant, but this is partly offset by the fact that many materials in this infrastructure are expected to be recycled when the plant is dismantled. This mitigates the life-cycle impact. The environmental relevance of infrastructure is closely linked to the relatively low ethylene yield by the plant.
- The role of energy consumption in the life-cycle impact is also relevant, quantified at 5.4 kWh/kg ethylene, assumed to be supplied by the grid. This aspect is ranked third in terms of GHG emissions related to plant operation, after electrolyte supply and carbon dioxide supply.
- The choice of photoanode material to be used in the PEC, namely $BiVO_4$ or $TiFe_2O_5$, seems to have very low influence on the overall life cycle impact of ethylene production by LICROX. This is mainly due to the fact that these materials are used in very low quantities.

1.7 Limitations of the study

At this stage, the LICROX consortium knows too little about what a commercial LICROX production plant will look like, which has led in this study to a general lack of primary data on many aspects, such as production of many underlying materials used in the PEC, infrastructure of a LICROX plant, energy consumption by such a plant, etc. This has been overcome with expert judgement by the consortium and 2.-0 LCA consultants, filling all gaps with the most appropriate available information. In spite of this, the uncertainty in the results is high: aspects that are judged in the results as having low priority could be in reality more important, and vice versa.

1.8 Recommendations

- In order for the LICROX technology to reduce its life-cycle impact, the most important identified parameter to improve is the ethylene yield by the PEC (in kg /m^2 PEC/day). Doubling this yield effectively halves the impact of many activities on a per kg ethylene basis. Other measures aimed at reducing this impact, in order of importance, are: reducing the electrolyte replacement frequency, using unprocessed flue gases as source of carbon dioxide, and the use of photovoltaic electricity to operate the plant. Nevertheless, the technical feasibility of implementing such improvements needs to be ultimately confirmed by the LICROX consortium.
- To conduct a theoretical scale up of the LICROX prototype that includes all unit operations expected in an industrial production plant, to validate this study. Such a scale up could be used as the basis for a more reliable application of LCA.

C. Ethical and societal consequences

Based on the findings of the prospective life cycle assessment, this chapter delves into societal consequences of the LICROX technology, noting that societal and ethical concerns may be conflated when relating them to emerging energy technologies. The exploration is based on stakeholder engagement carried out between June and September of 2022 and this chapter presents the results of two distinct workshops, both feeding into conclusions on societal consequences and steps to be taken in the field of PtX.

1. Understanding ethical and societal consequences of emerging energy technologies

Evidently, the development and implementation of new energy technologies is necessary for Europe to live up to the ambitions of the European Green Deal. This prioritization has direct and tangible consequences for the livelihoods of European citizens. For one, the choice to allocate vast resources to develop new technologies, is a matter of prioritization that will leave other sectors with weaker financing. While the necessary prioritization of resources is not a new or particularly problematic issue, it is important to be mindful that it is a zero-sum game. More importantly, however, we may focus our attention on the future European society that emerging energy technologies will have a considerable influence on. European livelihoods are, despite lacking awareness hereof, incredibly affected by (1) energy consumption manners and (2) the immediate landscape of citizens.

With the 2022 Russian attacks on Ukraine and the subsequent energy crisis, energy consumption has become more evident across Europe. Our dependency on (artificially) scarce energy sources have stressed the obvious fact that energy has to come from somewhere and that it can be taken away from us. A future European society that is run by renewable energy will need to be crucially aware as to where its energy is coming from and how a stable energy supply is secured for all citizens.

The fact that energy has to come from somewhere will be made abundantly clear with the transition to renewable energy, when current sources of oil, coal, and natural gas, will be replaced by windmills, photovoltaics, and PtX-plants. These large-scale infrastructural projects require space in Europe and will compete with other interests of land use, such as agriculture, biodiversity conservation, and housing. An exemplary study conducted by the Danish Board of Technology and Aalborg University (Arler et al., 2017) showed how Danish national and regional plans for land use exceeded the total area of Denmark, requiring approximately 130% of existing land. Lacking European awareness of the future landscapes we are forming will eventually affect citizens, when we have to prioritize between food, housing, energy, nature, and many other concerns.

It is clear that the implementation of a future energy technology like LICROX will influence European livelihoods directly. This prompts considerations and exploration of societal and ethical consequences and ways to circumvent risks. Societal and ethical concerns are effectively all concerns about livelihoods when it comes to the matter of energy technologies. They are, however, approached from different angles:

- Ethical concerns stem from normative idea of European democratic values and ambitions of a deliberative society. Essentially, policy choices that affect citizens should be aligned with citizen needs because it is a fundamental democratic right of Europeans.

- Societal concerns cover ethical concerns, but additionally includes the pragmatic notion that European citizen hold a great power to influence the implementation of energy technologies. When European livelihoods are threatened, civil mobilisation against said threats has proven

> an effective and strong response. Noteworthy examples could be the yellow vest protests initiated in France 2018, or, more explicitly, the Lützerath occupations initiated in 2020, currently hindering the expansion of brown-coal infrastructure. Citizen opposition is also mobilised in the implementation of renewable infrastructure, despite an overall societal goodwill (Rand and Hoen, 2017). Citizens care about their livelihoods and perceived threats to human security will be acted upon. For this reason, engagement of citizens in the sustainable transition is not just democratically important – it is essential to reduce societal resistance and ensure a successful implementation.

How then, do we engage society in the matter of emerging energy technologies? Boudet (2019) provides a useful insight to public perceptions of - and responses to technologies, like LICROX. One key message of the meta-study is that public familiarity with emerging energy technologies is very limited. While that in and of itself is not particularly surprising, related conclusions are important to take note of: Within the field of PtX, and energy technologies in general, the scientific literacy model (i.e., public opposition against technologies stem from lacking knowledge) is a popular assumption on societal barriers. However, Boudet concludes that such a model is much too reductionistic and that "knowledge is not a panacea for improving public understanding and encouraging informed discussions of energy technologies" (2019, p. 2). In fact, a myriad of factors influences public perception and responses to emerging technologies, as summarized in figure 19.

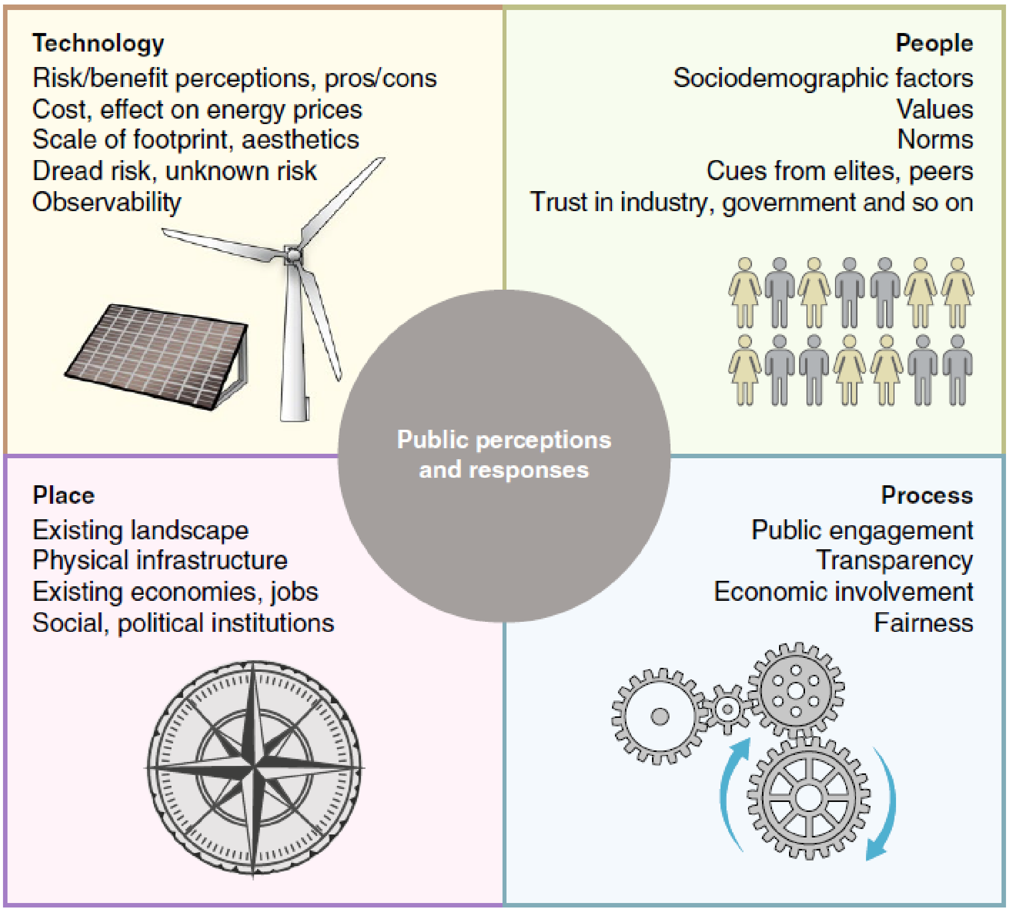


Figure 1. Factors affecting public perceptions of and responses to new energy technologies (Source: Boudet, 2019)

Evidently, PtX and direct solar conversion projects, and the overarching European effort to develop new energy technologies will benefit by exploring and planning within the four identified aspects of emerging technologies. In LICROX, people's perceptions will be partly explored in D6.4 *Societal acceptability*. However, cues from elites and peers may be identified by stakeholders, who hold knowledge on the field of energy and emerging technologies. Likewise, stakeholders from the fields of research, policy, and industry may provide useful insights to the aspects of technology, place, and process. Naturally, the scale of the LICROX project does not allow for a European-wide investigation covering all relevant aspects fully. However, this may prove a first useful step toward an increased knowledge and informed decision making on the four aspects identified. It is clear, already from the outset of this investigation, that inclusive deliberation and long-term strategies at an EU-level is needed to address public perceptions and responses to the emerging energy technologies.

The exploration of societal and ethical consequences of the LICROX technology is inherently limited. As has been made clear, the European public has very little familiarity with emerging energy technologies. Engaging society on a technology that is still at a rather low TRL, is difficult as the public knowledge and interest in the subject matter will be limited. Ironically, this is the stage where public involvement is especially important, as the ability to influence technological development is at its highest.

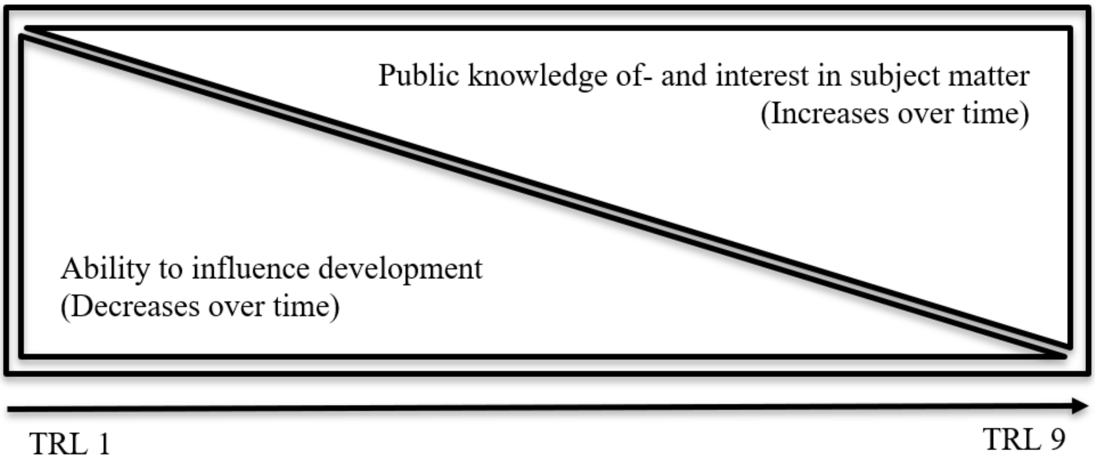


Figure 2. Illustration of the inverse relationship with influence and knowledge in emerging energy technologies

Once again, this means that the assessment of societal concerns that will be laid out in LICROX will focus on the broad strokes of emerging energy technologies and provide pointers for technological development. The exploration of the subject matter has been carried out in two major steps: First, stakeholders knowledgeable on the societal impact of solar fuel technologies have been engaged to lay out fundamental pointers for the rest of the exploration. Second, stakeholders knowledgeable on the development, exploitation, and societal and political implementation have been engaged to pinpoint specific barriers to the LICROX technology and the general development of comparable technologies. Both efforts of engagement have been carried out through discussion on societal consequences of LICROX, based on the notion that societal consequences are directly connected to policy- market- and social barriers to implementation of the technology.

2. Setting a framework for understanding societal and ethical energy issues

To set out the fundamental pillars for an exploration of societal and ethical consequences of the LICROX technology, a think-tank was established as part of the SUNERGY Initiative Roadmapping Workshop, held on June 14-15th of 2022. The workshop was facilitated under the framework of the European-funded SUNER-C CSA (Coordination and Support Action), aiming to bring together a range of portfolio projects to discuss the future of solar fuels and solar chemicals. The Danish Board of Technology facilitated a think-tank on social acceptability and the societal contract, engaging other projects, the EIC, and SUNERGY supporters to discuss societal and ethical issues of solar fuels and solar chemicals.

2.1 Method

The think-tank was carried out with a typical roadmapping exercise in mind, playing on the overarching theme of the SUNERGY workshop. The setting was facilitated following the world café method (Engage2020, 2014), aiming to mix opinions and knowledge at a rapid rate, to ensure generalizable outcomes.

The think-tank was initiated by setting a scene, where societal and ethical concerns need to be strengthened in the realm of emerging technologies. Participants were asked to reflect on the fact that societal concerns are not explicitly and systematically included early in the development process of new technologies. The prompt of the think tank was thus presented as the following:

The problem: Technological development lacks early and frequent consolidation with society
Technological innovation is in a mutual relationship with society. As society shapes the context within which technology is developed, new technologies alter people's lives and society as a whole. Unfortunately, technological roadmapping can, more often than not, come to view this relationship from a one-sided perspective: New technologies are what drive change in society and it is thus the task of researchers to know what to develop and how to do so. When we look back at the history of technological development, this understanding is misleading; technological innovation is inherently entangled with societal concerns and cannot be driven well without an understanding of this entanglement. Our constantly changing society affects innovation, and roadmapping processes need to reflect this fact.

Developers and researchers may be familiar with the situation where a technology has been developed over several years and time has come for it to be put on the market. For some reason, however, the societal response to a new technology may not be as positive as expected. Many technological projects are parted into an initial development phase, followed by a social acceptability phase, during which barriers to implementation are sought to be overcome. Time and effort is wasted when innovation is not guided properly toward the society it aims to reach. This problem can, however, be addressed. Innovation processes that succeed in engaging with society early and frequently are much more likely to develop technologies and products that flourish on the market and respond to societal needs. While societal engagement is not an easy or automatic fix for every problem, practiced engagement often leads to (1) knowledge being raised, (2) opinions being formed, and (3) actions being initialised.

Based on the prompt, participants were asked to consider the integration of societal concerns in the development of novel energy technologies. These considerations were stimulated by providing three angles, from which participants could form their arguments:

1. *Fundamental rights and ethics*
   Novel energy technologies stand to transform the European energy landscape and thus the lives of millions of citizens. How may innovation and implementation processes integrate fundamental rights and ethics to minimize negative impacts on livelihoods?

2. *Societal conflicts of interest*
   Interests in land use, economic benefits, and energy politics are seldom automatically aligned. How may societal conflicts of interest be made foreseeable and addressed in the development of novel technologies?

3. *Rational decision-making*
   Silver bullets don't exist, and policymakers and regulators alike will need to make informed choices in the development of the emerging energy landscape. How can novel technologies contribute to a fair distribution of cost, risks, and benefits?

With the scene prompted and the three angles for discussion, participants were mixed in groups that discussed their views, switching up the group constellation at fixed intervals, to ensure a multitude of views for all points raised.

2.2 Results

The first session of the think tank provided a deeper insight into the three angles established in the preparation material. During the discussion, participants were asked to write down points of interest on post-its, placing the note near other notes with similar points. In this way, an affinity diagram emerged for each angle, providing an overview of themes that would be important to consider. For example, under the angle of rational decision-making, several notes pointed toward an issue of information. *What information is necessary to make rational decisions? How may citizens receive and give information that aids decision-making? How is scientific evidence, policy development, societal concerns, and other types of relevant information processed and prioritised?*

Altogether, nine clusters emerged under the three angles provided in the preparation material. During the second session of the think tank, participants were prompted to delve into each cluster, discussing potential recommendations for action. The discussion was shaped through templates (see figure 1) which required consideration on the nature of the issue, relevant people to involve, the level of involvement (regional, national, EU-level, global), as well as an indication of time of involvement. For the latter, two timelines were provided: (1) An abstract visualisation of the policy cycle and (2) a general timeline of technological innovation.

In this way, all nine clusters were discussed, and participants were pushed to explore how societal concerns may be thought into technological innovation processes, as well as the SUNERGY initiative. While this exercise proved but a first step towards increased societal engagement in the emerging field of novel S2F-technologies, three overarching conclusions were made:
1. Solar-to-fuel technologies can gain credibility, momentum, and resilience if society is engaged already in the agenda-setting of a project.
2. Solar fuels hold great power to disrupt the future energy market. Decision-making and innovation management need to be informed by scientific evidence, political momentum, and societal concerns.

3. Societal engagement is important, but difficult to carry out, especially in highly sophisticated technological development. Reliance on experts in societal engagement and societal technology assessment is key.

3. Exploring societal and ethical consequences with stakeholders

With the three overarching conclusions on solar fuel technologies, it was possible to set a direction for the exploration of societal and ethical consequences of LICROX. The nature of this exploration was more tangible, aiming to form a concrete vision for the technology, and identifying barriers and solutions for this vision. In this way, we could form the necessary next steps, not only for the project, but for the general development of solar fuel technologies.

3.1 Method

To pursue said aim, the DBT facilitated a future workshop with selected stakeholders. The future workshop is a method of engagement designed specifically to define aims and identify problems by relevant stakeholders (Engage2020, 2014). In practice, this is carried out in three phases, providing LICROX with three critical outcomes: (1) critical perspectives on LICROX, (2) a scenario for LICROX in 2040, and (3) barriers and solutions to reach said scenario.

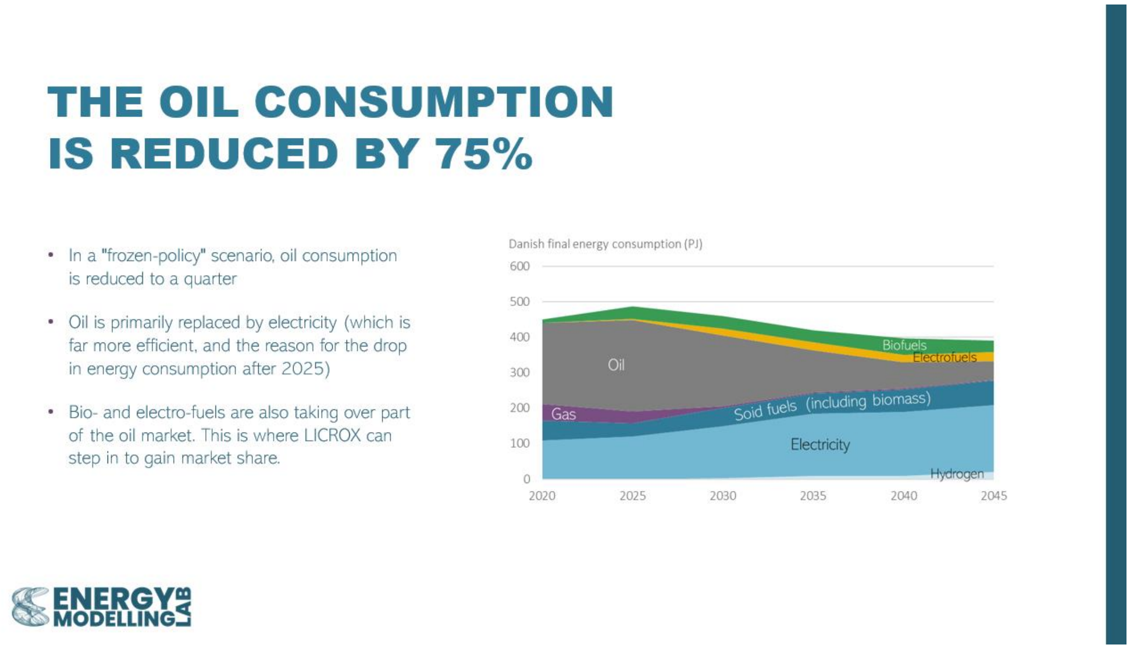
1. Critical analysis: During the first phase of the workshop, the technology at hand is discussed and analyzed critically from several perspectives. These perspectives lead on to an open discussion among stakeholders, providing both knowledge for input and points for contention.
2. Vision building: The second phase of the workshop builds on the critical analysis and applies the perspectives discussed to develop a future vision of the technology at hand. The vision is deliberated and reality checked to ensure that it is built upon plausible presumptions and identified trends. The final vision may consist of a scenario for the technology, which becomes the focal point for the final part of the workshop.
3. Identifying actions: The final phase of the workshop sets out from the future scenario for the technology, aiming to make it tangible. It does so by identifying barriers between the current status of the technology and the future scenario. These barriers are then discussed with the aim of identifying actionable solutions. In this way, the immediate next steps for the technology are identified and explored by knowledgeable stakeholders.

3.2 The workshop

1. Critical analysis

During the workshop, this first phase was carried out with the help of three keynote speakers, to ensure that the analysis included critical perspectives that helped stakeholders discuss LICROX in a nuanced manner. As laid out at the beginning of this report, much of the actual implementation of PtX-technologies has yet to be tangibly discussed and planned. The three critical perspectives provided a way for stakeholders to consider actual issues that may arise during the implementation of a LICROX technology in Europe. The three perspectives are outlined as follows:

First, Mr. Kenneth Karlsson, with assistance of Ms. Alexandra Freltoft (Energy Modelling Lab, DK) shared a projection of the future energy market. Based on the prospective energy landscape modelling of Energy Modelling Lab, we were able to paint a picture of the future energy market of 2040-45. It was made clear how the market for e-fuels is growing, but not at a rate comparable to that of electrification.



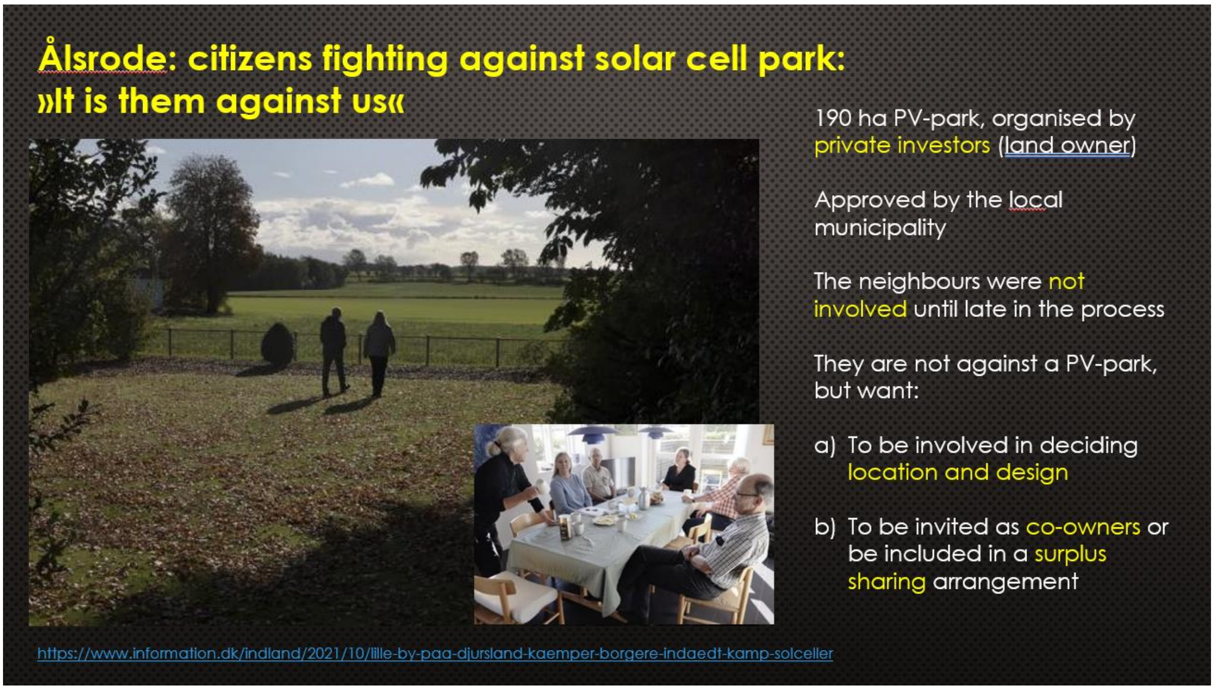
THE OIL CONSUMPTION IS REDUCED BY 75%

- In a "frozen-policy" scenario, oil consumption is reduced to a quarter
- Oil is primarily replaced by electricity (which is far more efficient, and the reason for the drop in energy consumption after 2025)
- Bio- and electro-fuels are also taking over part of the oil market. This is where LICROX can step in to gain market share.

Figure 3. Highlight from presentation by Mr. Kenneth Karlsson

It was also stressed that the improvement rate of batteries should not be underestimated and that the market of e-fuels depends on the efficiency of large-scale batteries. This led to the conclusion that technologies like LICROX may benefit from a focus on the chemical and biochemical sector for a future market, as plastics and pharmaceuticals will rely on a carbon-neutral ethylene input. Last, it was made clear how infrastructure for PtX-plants, as well as the additional renewable energy sources that are necessary to power the plants, will affect the European landscape.

The issue of infrastructure was expanded by the second keynote speaker, Mr. Finn Arler (Aalborg University, DK), who shared experiences with the practical implementation of energy infrastructure. His research points toward the necessity of democratic procedures when planning energy infrastructures, as failure to do so may result in debilitating societal resistance.



Ålsrode: citizens fighting against solar cell park: »It is them against us«

190 ha PV-park, organised by private investors (land owner)

Approved by the local municipality

The neighbours were not involved until late in the process

They are not against a PV-park, but want:

a) To be involved in deciding location and design

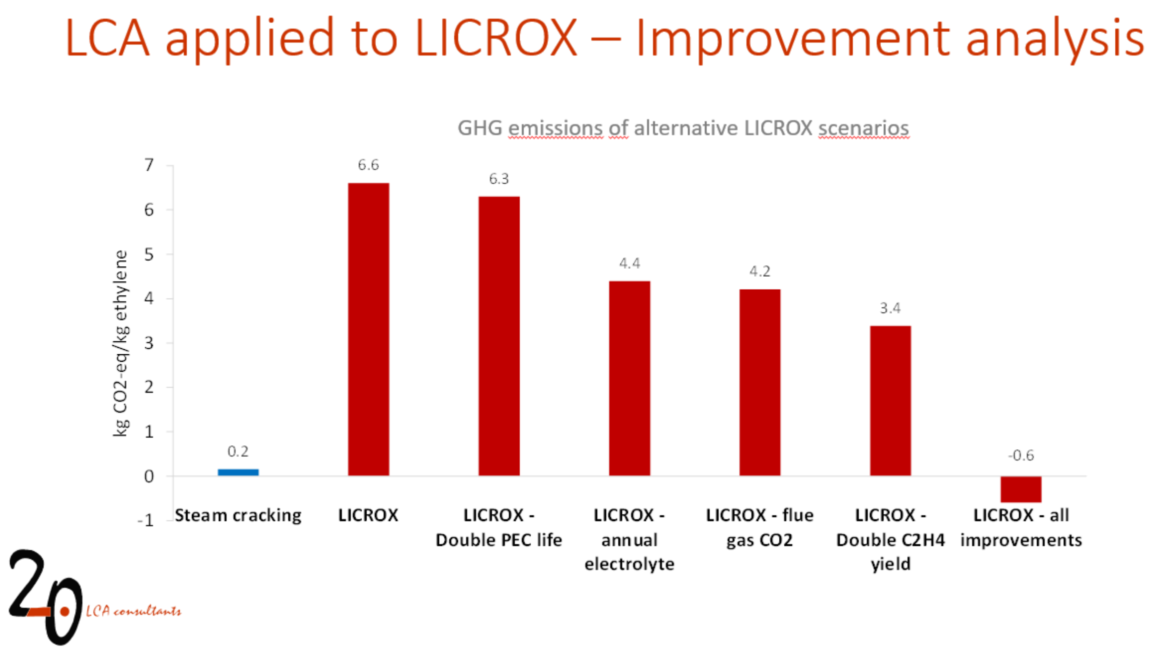
b) To be invited as co-owners or be included in a surplus sharing arrangement

https://www.information.dk/indland/2021/10/lille-by-paa-djursland-kaemper-borgere-indaedt-kamp-solceller

Figure 4. Highlight from presentation by Mr. Finn Arler

This second presentation made it clear how the practical implementation of the necessary infrastructure could become a major barrier for LICROX and other PtX-technologies, if plans for societal inclusion are not laid out early in the process. While it was stressed how inclusion of citizens in the planning and financing of renewable energy projects is important, it was also highlighted how researchers could factor in multi-functionality in the design of their technology, to minimize societal resistance.

An input aimed at the technology was the focus of the third and final keynote speaker, Dr. Ivan Muñoz (2.-0 LCA Consultants, DK). His presentation laid out the key messages of the LCA presented in section B of this report, indicating the work that is yet to be done to develop a technology favorable to conventional ethylene production methods.



LCA applied to LICROX – Improvement analysis

Figure 5. Highlight from presentation by Dr. Ivan Muñoz. Note: updated results with an improved method show higher GHG emissions for steam cracking, 1.4 and slightly less for the different LICROX scenarios (5.4 for LICROX -0.8 for LICROX-all improvements), these does not affect the general conclusions of the report.

The final presentation stressed how design choices in LICROX may critically influence the environmental consequences of the technology. It was made clear how material dependencies of a technology may become critical and influence its eventual implementation. The presentation spurred thoughts about the future deposits of all sorts of materials, from CO_2 to fresh water.

The three presentations laid the foundation for a discussion among stakeholders, who found points of contention among each other in all three (and other) arenas. The input successfully spurred a critical analysis of LICROX and solar fuel technologies in general, highlighting the many different points of view that exist in the field.

2. Vision building

Based on a discussion of the three perspectives, participants were able to identify key trends and characteristics of a future scenario for technologies like LICROX. By voting on the most viable characteristics, participants were able to prioritize and provide a weighted input for the Danish Board of Technology (see figure 24).

The exercise allowed for an informed scenario building of a European reality in the year 2040, which provided a tangible focal point for a discussion of LICROX and solar fuel technologies. The scenario constituted a realistic proposal of which role solar fuel technologies should play in Europe in 2040.

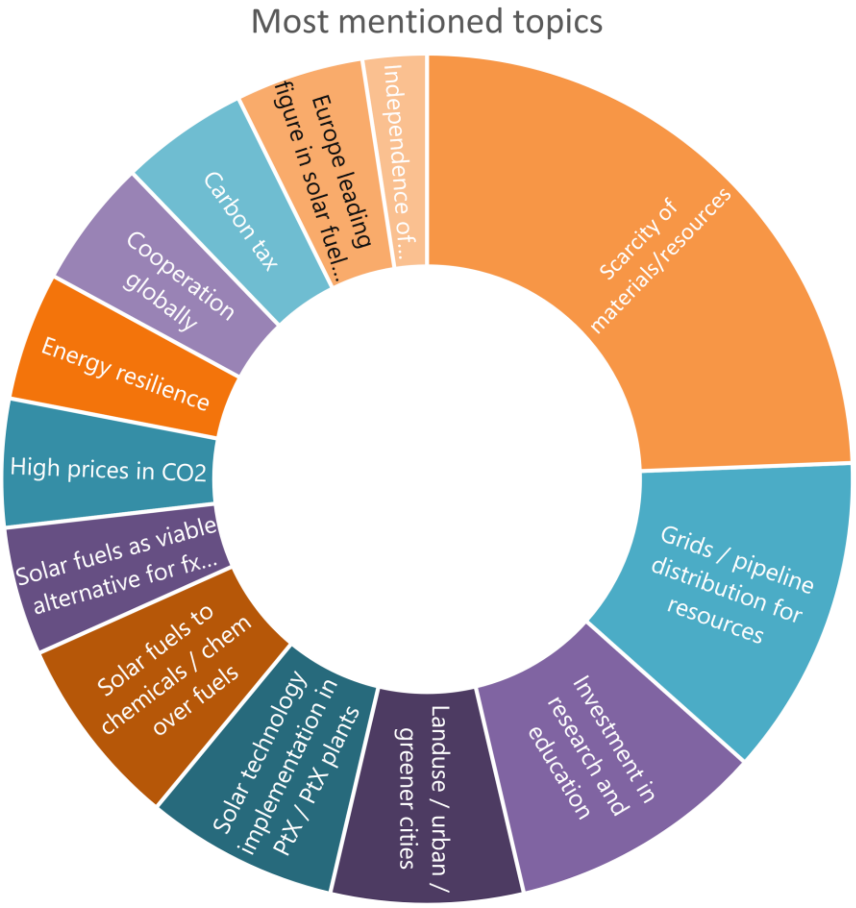


Figure 6. Weighted characteristics of a future scenario

Synthesizing the scenario into five key points, the participants were left with the following foundation for their discussion:

- Europe is a leading figure in technologies like LICROX, and a few hundred PtX plants are implemented, producing primarily chemical feedstock (potentially also fuels)
- Resources like minerals, water, CO_2, and area are scarce and sourcing is non-stable
- CO_2-emissions have become considerably more expensive
- Europe has increased its energy resilience and sovereignty, having implemented the necessary infrastructure for transportation of StF (Solar to Fuel) materials, being able to store energy chemically
- Urbanization has continued, leading to great geographic variations in energy needs

3. Identifying actions

With the scenario as a basis for discussion, participants were guided through exercise, aiming at identifying barriers and solutions related to the LICROX scenario. To focus the discussion, participants were parted into three groups, each focusing on one of the three perspectives brought in at the beginning of the workshop.

Barriers and solutions related to the future energy landscape

The participants focusing on the future energy landscape identified three barriers for the future of LICROX, based on the scenario given:

1. **Policy and regulation** were seen as a barrier because of the lacking consistency in the field of energy. Participants discussed the inherent problems of modern democracy and its conflict with technocratic solutions, specifically highlighting an issue with unelected specialists and policymakers. A general uncertainty and lack of vision leads to little investment and public support of solar fuel technologies.
2. **European lifestyles** were seen as a barrier because consumers are seen as rational beings that will choose the cheapest energy option. Consumers seem to think that energy should be cheap, even free, which does not harmonize well with the future energy landscape where energy will be much more expensive, and CO_2 will be a commodity.
3. **Technological complexity** was seen as the final barrier for solar fuels, both today and in 2040. Lacking public understanding of complex technologies were seen as a primary reason for lacking support in technologies like LICROX. Solar fuel technologies like LICROX are multidisciplinary and reliant upon complex chemistry, which makes societal support, and ultimately, funding difficult.

For each of the three barriers, participants identified several potential spaces for solutions.

Policy and regulation – Solutions

- Implementing a role of a long-lasting scientific officer, who could increase consistency in regulation and policymaking.
- Involvement of scientists in policymaking should be institutionalized, aiding policymakers in making evidence-informed decisions.
- Engagement of citizens is vital in strengthening the science-society-policy interface. Engagement practices of northern Europe should be carried out in southern and western Europe as well.
- Regulation and policies should be implemented that actively encourage a sustainable transition (e.g., taxing of carbon emissions, funding for research)

European lifestyles – Solutions

- Europeans should be educated on the topic of energy end energy technologies.
- Research on solar fuel technologies should continue, hopefully increasing efficiency.

Technological complexity – Solutions

- An energy council, working at a national or European level should be implemented to increase transparency and aid political understanding of solar fuel research.
- Complex chemistry should be targeted in informational campaigns to increase understanding and interest in the field that influences energy technologies.

Barriers and solutions related to practical implementation

The participants focusing on practical implementation identified three barriers for the future of LICROX, based on the scenario given:

1. **Technology** was seen as a barrier because the LICROX technology is complex and difficult to understand for policymakers, investors, and citizens alike. The technical complexity also makes it difficult to scale-up and prototype the technology.
2. **Policy** was seen as a barrier, concluding that there is a need for strong EU leadership and long-term planning across EU on the energy landscape. The solar fuel technologies need to be prioritized in the long-term planning to develop into a full scale market-ready technology.
3. **Investment** was seen as a barrier because it is difficult to find private investors that want to take the risk and fund the upscaling of the technology, which contains the technology to the lab. There needs to be a clear business case, which aligns with the long-term planning in policy.

For each of the three barriers, participants identified several potential spaces for solutions.

Technology – Solutions
- Pushing the scale-up of the LICROX technology and subsequent projects, eventually forming investments and policy changes.
- Subsequent project applications should include a focus on EU regulators as a recipient of recommendations within the field of novel solar fuel technologies.
- A closer relationship between EU project owners and funded projects is needed to get a better understanding of the fields and be able to create communities within the solar fuels.
- Increasing public control of patents, through funding of public research projects.
- Strategic foresight should be applied in policymaking to determine long-term suitable areas in Europe where energy technologies may be implemented.

Policy – Solutions
- Stronger European leadership is needed to make strategic and long-lasting decisions for a fair, equal sustainable transition, specifying the expected role of energy technologies.
- Programs that integrate society into the scientific community should be strengthened.
- An increased focus on energy, climate, and EU treaties is needed.
- Strengthening cross-cooperation between actors in the field of solar fuels.

Investments – Solutions
- Fast tracking investments in the needed technologies activating both private and public investments. Private investments should be targeted on the market ready technologies, and high-risk investments should be supported by public.
- Continuous investment in public communication and dissemination of these technologies.
- Strong and stable legal frameworks providing transparency. Tax incentives on solar fuel investments.
- Investing in securing the right labor markets and skills, securing future skills and competences when implementing.

Barriers and solutions related to resources and materials

The participants focusing resources and materials identified five barriers for the future of LICROX, based on the scenario given:

1. **The dispersion of scarce materials** (both geographical and geopolitical) was seen as a barrier, as it highly influences capital expenditure, potentially hindering scalability of the technology. As such, the economic and ecological viability of the technology is limited, minimizing exporting possibilities.
2. **Land availability** was seen as a barrier, as energy demands are continuously rising, but energy production, which requires land has a natural cap. Additionally, the LICROX technology was seen to be dependent on point sources, both in terms of acquiring carbon, but also in terms of distributing an output. This makes deployment difficult and potentially expensive.
3. **Fresh water** was seen as a barrier, as clean water will be a contested resource, which could threaten societal acceptance of the technology.
4. **CO_2** was seen as a barrier as it is expected to become an expensive commodity in the future. Because the LICROX technology currently is dependent on commercial CO_2, the expectation is that the market will be difficult to penetrate.
5. **Technological competition** was seen as a barrier, as other technologies with a higher TRL may stand in the way of technological development, as investments are limited.

For the top four barriers, participants identified several potential spaces for solutions.

Dispersion of scarce materials – Solutions

- At a technological level, researchers should aim for increased stability of the LICROX PEC, as well as an easy implementation of the final technology.
- At a societal level, increased knowledge building on climate change was seen as necessary to understand the role of energy technologies and the societal prioritization that comes along with them.
- At a policy level, stability was the primary focus, suggesting that a list of non-critical materials, that would be applicable for a minimum of 10 years would improve research. Alongside this, increased funding for research was mentioned. Last, a political focus on self-sufficiency, potentially opening up the notion of European mining was explored.

Land availability – Solutions

- At a technological level, researchers should explore pathways for increased productivity, and engineers should explore pathways for integrated solutions.
- At a societal level, inclusion and co-involvement of land-use planning was seen as a viable pathway for long-lasting energy solutions.
- At a policy level, transparent and inclusive prioritization of land use was highlighted as a space for solutions.

Water competition – Solutions

- At a technological level, researchers should explore potentials for wastewater purification in connection with the LICROX PEC, as well as the potential of increasing resistance to contaminants in the PEC.
- At a societal level, water saving solutions should be implemented broadly, alongside clear dissemination efforts in showing how the LICROX PEC does not compete with drinking water, if it manages to use purified wastewater.

- At a policy level, the EU should set out an ambitious water use policy, clarifying societal prioritization and providing stability for further research. To some extent, water use should be regulated as well, to minimize competition.

CO_2 – Solutions

- Industries could explore potential synergies with LICROX technology capturing carbon emissions at the source, providing a direct input for the industry. Especially the plastics and biochemical industry, where ethylene is a necessary input, such pathways could be viable.

3.3 Concluding thoughts on societal and ethical consequences

The stakeholder workshops in LICROX provided crucial outcomes on two levels: First, at a project level, where outcomes should be integrated in the development of LICROX, as well as follow-up projects. Second, at a societal level, where needs for political and structural changes are identified.

Project-level recommendations and thoughts

The LICROX PEC may improve considerably by aiming to reduce the life-cycle impact.

The LCA points to four technological goals for the LICROX PEC to reduce the life-cycle impact. The main goal is to increase the ethylene yield by the PEC, i.e., improving efficiency. Secondary goals are, in order of importance, to reduce the electrolyte replacement frequency, using unprocessed flue gases as a source of carbon dioxide, and using photovoltaic electricity to operate the plant. Reaching these benchmarks will strengthen the LICROX technology considerably, not only from an LCA-perspective, but for marketability and societal acceptability.

The market for sustainably produced ethylene may primarily be found in the chemistry sector.

While the LICROX technology is framed as a solar fuel technology, it may be useful to explore exploitation within the chemistry sector. The stakeholder workshop in Copenhagen pointed toward lacking technologies to produce commodity chemicals sustainably, while more competition exists within the field of solar fuels, hydrogen dominating this sector.

Overarching recommendations and thoughts

Both stakeholder workshops clearly indicated that the field of solar fuels, even that of Power-to-X, is affected by conflicting interests and knowledge. The LICROX technology is at the frontier of novel energy technologies, thus uncertainty about development paths is a natural occurrence. What we may gather from the stakeholder workshops are indicative concerns and issues that relate to the general development of solar fuels. However, further investigation is necessary to continue the mapping of these and currently unknown concerns. At this stage, the stakeholder engagement points to four crucial overarching areas that need to be explored further.

Citizens need to be engaged in international and local energy infrastructure planning.

It is increasingly becoming clear that the involvement of citizens at all levels of planning and development is crucial for a sustainable transition. This need goes beyond normative ideas of European democratic values and ambitions of a deliberative society; involving citizens in transitions has clear pragmatic merits. Citizens that are feeling left out of societal decision-making may play a strong opposing role on new implementations, as has been seen with several sustainable energy infrastructure projects (Rand and Hoen, 2017). On the other hand, citizens that are engaged in local energy infrastructure projects may benefit from their own engagement, turning them into a strong advocate for the transition to sustainable energy (Jørgensen et al., 2019).

The engagement of citizens should be carried out at two levels of the sustainable transition. First, at the agenda-setting: What kind of energy landscape do citizens want in the future? The EC has already shown commitment to these kinds of efforts with the facilitation of the Conference on the Future of Europe (2022). The conference identified the concerns of European citizens in terms of climate change and energy use, stressing a need for European energy security and energy independence in ensuring a just transition. Notably, citizens stressed a need for investments in renewable energy and energy efficiency as the primary objectives for the transition, but also indicated a necessity of new technologies for the sectors that are difficult to electrify, highlighting green hydrogen. Enabling citizens to pave the way for technology development and sustainable transitions is crucial to achieve fair processes and subsequent societal acceptability (Boudet, 2019).

The second level is that of technological development, in projects like LICROX. The stakeholder workshops, however, indicated that involving society and citizens at an early stage in technology development is a challenge as it demands technological understanding and capabilities. In order to overcome this challenge, we recommend to translate technological development to its outputs that are relatable to citizens. For the case of energy, fluctuations in price and supply are the primary phenomena that makes energy ‘visible’ to citizens (Boudet 2019). Translating new technologies into a new energy landscape, where prices and supply may be different is a useful way to engage citizens. This is the approach carried out in T6.2, where the method EuropeSay is applied. EuropeSay is a deliberative method, a mix between focus groups and surveys facilitated by an online platform. The LICROX consortium, with DBT in charge will use this tool to perform citizen’s workshops, to be undertaken in 5 different European countries. The objective is to provide early engagement, reaching several hundred citizens. The results of the engagement study will give an indication of the citizens' perceptions of LICROX on a range of issues such as land use, resources and economics. Building on top of this approach to investigate more societal concerns in a European-wide scope, is recommended to strengthen the understanding of societal acceptability.

Long-term, inclusive energy policies with clear strategies for Power-to-X need to be laid out.

One of the overarching conclusions from the think tank was that solar fuels hold great power to disrupt the future energy market. This was also a discussion point in the future workshop, where many of the stakeholders pointed out that this disruptive nature also calls for long-term planning. Scientists stressed that the changing policy field made it difficult to carry out good scientific practice and progress. Using citizen’s engagement to set up a clear framework for a future European energy landscape would provide citizens and scientists with clarity and useful objectives. Building on top of efforts in CoFE (2022) and FETA (2022) will strengthen such a framework.

Stable and strategic investments in a societally desired energy landscape is needed.

The transition to renewable energy requires investments at several levels. From the stakeholder engagement it was made clear how investments are necessary to: (1) provide a stable ecosystem for technological development; and (2) ensure democratic processes at the implementation of solar fuel technologies. Naturally, such investments require long-term, sector cross-cutting planning based on European values and citizen views.

A stable ecosystem for development was stressed by several stakeholders as a necessity to develop energy technologies that can compete with alternatives in terms of efficiency and economic viability, while adhering to societal needs. As emerging technologies like LICROX have yet to prove an existing market advantage, private investments are scarce, meaning that continued, even strengthened public investments are needed. In practice, this could be pursued through funding programmes as has been seen in H2020 and is emerging in Horizon Europe. Collaborative funding efforts, as exemplified by the SUNER-C CSA are also effective financially stabilizing efforts, which could be continued and strengthened. A strengthened involvement of the EIC in the development of research projects is recommendable.

As has been stressed above, policy and investment planning is dependent on effective engagement of citizens and stakeholders. Funding schemes may benefit from engaging academia as well as citizen’s perceptions, allowing future projects and initiatives to be shaped by existing needs funded in tacit knowledge. Taking pointers from the recently concluded Conference on the Future of Europe (CoFoE, 2022), may strengthen public investments, and ensure adherence to public values and concerns. Explicit investments are, however, still needed to strategically foresee and plan future European land use in an inclusive manner, including the infrastructure necessary for the transition to renewables.

In addition to the necessary investments in technological development, consistent and thorough buy-in on public dissemination and engagement regarding emerging energy technologies is essential to strengthen the European position in PtX-technologies. Additionally, investments can be made to incentivize and strengthen processes that fast-track technological development, such as tax incentives, and a future labor market and skills.

For the investments directly aimed at LICROX, the market potential has yet to be assessed. In the exploitation plan, expected to be delivered at the end of the project, concrete steps for the commercialization and exploitation of the technology will be laid out. As was outlayed in the stakeholder-built scenario, PtX-technologies producing a carbon-based output, like ethylene, may benefit from expanding their planned consumer base from fuel dependent actors, like transportation and heating. Potential expansion sectors could be high-end products, where chemical purity is of importance, like the biochemical industry, or rapidly expanding sectors with an unresolved need to minimize carbon emissions, like the plastics industry.

Development of novel energy technologies should seriously integrate concerns of diminishing resources, including freshwater and land areas.

The life cycle assessment and the subsequent discussion of its results among stakeholders concluded the very tangible need to raise awareness of future resource scarcity and realistic expectations for the potential of PtX-technologies. Although solar and wind energy is abundant, the technologies that convert these energies to a useful output for society need finite materials. While e.g., freshwater is not a scarce resource in Europe presently, coordinated foresight is necessary to identify the material dependencies that the future European energy landscape will be dependent on. Potential resource scarcity should be explored from both a real and artificial perspective, as European wishes to achieve energy independence has geopolitical consequences, which may cut off material influx.

European efforts to increase public understanding of energy use and its resource dependency is recommended. As was pointed out during the stakeholder workshop, no foreseeable technology can outbalance an ever-increasing energy demand. Once again, citizen’s recommendation on the energy sector laid out in CoFE(2022) are worth exploring further through deliberative methods.

D. Next steps

The findings presented in the report feed into two major tasks in the LICROX project. First, as described, the citizen’s engagement, where the EuropeSay method is applied to further explore topics identified with stakeholders. Second, the LICROX exploitation plan, where societal concerns stemming from the stakeholder workshops indicate the shape of a future market. For example, it has been clearly indicated that there may be a future market in the biochemical or plastics industry, which should be explored further.

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Annex A Life Cycle Assessment

Life Cycle Assessment of the LICROX technology

By Ivan Muñoz
2.-0 LCA consultants, Barcelona, Spain
22 November 2022

Preface

This report describes the life cycle assessment (LCA) of ethylene production through the photoelectrochemical cell technology developed by the LICROX consortium. A comparison is carried out with ethylene from petrochemical sources. The study has been commissioned by the LICROX consortium and this report has been prepared by 2.-0 LCA consultants from December 2021 to November 2022.

2.-0 LCA consultants, Barcelona, Spain

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Executive summary

The LICROX project

LICROX is a Research and Innovation Action project funded by the European Commission under the Horizon 2020 programme. The aim of the project is to produce and test a photoelectrochemical cell (PEC) for converting sunlight into organic molecules. Such organic molecules can then be used either as fuels or as platform chemicals. As part of the LICROX project, a life cycle assessment (LCA) study has been conducted, consisting of two iterations. This report describes the second and final iteration of the LCA study, following the ISO standards on LCA: ISO 14040:2006 and ISO 14044:2006. The study has been subject to a critical review by an independent external LCA expert.

Goal

The goals of this study are twofold:

- To assess the life-cycle impacts of the LICROX technology at an early stage of development, in order to identify key hotspots and suggest potential improvement options.
- To compare LICROX with a conventional technology to produce ethylene, namely petrochemical steam cracking.

Systems under study

The target product for the two production processes under study is ethylene, a hydrocarbon with the formula C_2H_4. The most common industrial process for production of ethylene is via steam cracking of crude oil-based feedstocks.

Steam cracking is a petrochemical process in which saturated hydrocarbons are broken down into smaller, often unsaturated, hydrocarbons. Steam cracker units are facilities in which a feedstock such as naphtha is thermally cracked through the use of steam in steam cracking furnaces. The main product from steam crackers is ethylene, but other valuable co-products are produced, such as propylene, C4 hydrocarbons such as butadiene, and pyrolysis gasoline, for example.

Production of ethylene by means of the LICROX concept is assessed considering a hypothetical industrial plant, with an unspecified production capacity, located in Europe. This plant includes the following elements:

- The PEC device, installed in a ground installation, in a similar fashion as in a photovoltaic plant.
- Structural support and piping.
- An ultrapure water production unit.
- A chemical dosing station, from which CO_2 and electrolyte (potassium bicarbonate solution) are supplied.
- Auxiliary devices such as pumps, control and monitoring system, sampling and gas analysis system.
- A downstream processing unit, which will mainly consist of a gas separation process by means of pressure swing adsorption.

The functional unit and reference flow used in the study to compare both systems are 1 kg ethylene. The study can be considered as a ‘cradle-to-gate’ LCA of ethylene, since the downstream stages of ethylene conversion to final products, their use and disposal are excluded. This is justified given that these life cycle stages are expected to be the same regardless of how the ethylene is produced, and therefore they become irrelevant from a comparative point of view.

Data sources and quality

All activities in the life cycle are ultimately linked in the background to the ecoinvent database, version 3.6, specifically the ‘Substitution, consequential, long-term’ system model.

Production of the PEC device and its underlying components is based on data provided by the consortium on the specific materials incorporated in the device. In many cases, specific inventories have been developed by 2.-0 LCA consultants for a substantial number of materials. These estimated inventories have a high uncertainty. Data on manufacturing the PEC (sputtering, roll-to-roll processing, thermal evaporation, gravure coating, encapsulation) have been compiled by the consortium partner ICFO, to reflect a real industrial process.

Data on the infrastructure needed to build a full-scale LICROX plant were not available. This has been covered with published data describing a solar-assisted photocatalysis plant treating industrial wastewaters in Spain. With these data we attempt to cover the requirements for civil engineering, structural materials, piping, etc. for a hypothetical LICROX plant, excluding downstream processing of the produced gases, the latter included as a pressure swing adsorption (PSA) process, covered by means of literature data on an industrial PSA plant treating biogas.

Data on operation of a hypothetical LICROX plant were equally scarce. A basic mass and energy balance for the overall process has been defined based on reasonable expectations by the consortium, basic stoichiometry, etc. Several key aspects were also suggested by the consortium as a best guess, namely the PEC useful life, the ethylene yield, the carbon dioxide utilization efficiency, the composition and replacement rate for the electrolyte, as well as electricity consumption by the whole plant. Regarding the carbon source, pressurized carbon dioxide from a nearby industrial source is assumed as the default scenario. Finally, the end-of-life stage for the LICROX plant assumes a plausible fate for each material, chiefly recycling/disposal.

Regarding steam cracking, a dedicated model for ethylene production by this technology has been developed. This required, in addition, to develop a model for production of propylene, the main by-product from steam cracking. Both models have been built based on published data on process simulation, providing a sufficiently detailed mass and energy balance for steam cracking using naphtha as feedstock, and for propylene production using methanol as feedstock.

Impact assessment method

The method used for impact assessment is ‘Stepwise’. In total, this method includes a total of 16 impact categories, which can be expressed in biophysical units (mid-point), and in a common unit expressing damage (endpoint), namely in monetary units.

Key findings

The main conclusions of the study can be summarized as follows:

- Life cycle impacts from ethylene produced by a hypothetical LICROX production plant, as envisaged in this study, appear to be substantially higher than those for ethylene produced by conventional steam cracking. This is the case for 15 out of the 16 indicators included in Stepwise. As an example, GHG emissions are 34 times higher for LICROX.
- The main driver for environmental impacts of the LICROX technology corresponds to plant operation. Two main aspects are highlighted as key contributors: electrolyte supply and CO_2 supply. The impact of electrolyte supply is closely related to the fact that potassium bicarbonate and ultrapure water need to be added and replaced on a weekly basis, while the impact of Carbon dioxide supply mainly corresponds to the energy use associated to recovering this gas from industrial exhaust gases.
- The environmental impact associated to the PEC as a component of the LICROX plant is not negligible. It can be considered as the second most important aspect after plant operation, and this is closely related to the relatively low ethylene yield. The environmental impact of the PEC is highly dependent on the assumed useful life, which has been taken as 10 years. However, this degree of durability is currently more a hope or a goal than a fact. The main identified contributor to the environmental impact of PEC as a component is the electricity consumed during its manufacturing.
- Other plant infrastructure construction and disposal (including the downstream processing unit) appear to also be relevant, but this is partly offset by the fact that many materials in this infrastructure are expected to be recycled when the plant is dismantled. This mitigates the life-cycle impact. The environmental relevance of infrastructure is closely linked to the relatively low ethylene yield by the plant.
- The role of energy consumption in the life-cycle impact is also relevant, quantified at 5.4 kWh/kg ethylene, assumed to be supplied by the grid. This aspect is ranked third in terms of GHG emissions related to plant operation, after electrolyte supply and carbon dioxide supply.
- The choice of photoanode material to be used in the PEC, namely $BiVO_4$ or $TiFe_2O_5$, seems to have very low influence on the overall life cycle impact of ethylene production by LICROX. This is mainly due to the fact that these materials are used in very low quantities.

Limitations of the study

At this stage, the LICROX consortium knows too little about what a commercial LICROX production plant will look like, which has led in this study to a general lack of primary data on many aspects, such as production of many underlying materials used in the PEC, infrastructure of a LICROX plant, energy consumption by such a plant, etc. This has been overcome with expert judgement by the consortium and 2.-0 LCA consultants, filling all gaps with the most appropriate available information. In spite of this, the uncertainty in the results is high: aspects that are judged in the results as having low priority could be in reality more important, and vice versa.

Recommendations

- In order for the LICROX technology to reduce its life-cycle impact, the most important identified parameter to improve is the ethylene yield by the PEC (in kg /m^2 PEC/day). Doubling this yield effectively halves the impact of many activities on a per kg ethylene basis. Other measures aimed at reducing this impact, in order of importance, are: reducing the electrolyte replacement frequency, using unprocessed flue gases as source of carbon dioxide, and the use of photovoltaic electricity to operate the plant. Nevertheless, the technical feasibility of implementing such improvements needs to be ultimately confirmed by the LICROX consortium.

- To conduct a theoretical scale up of the LICROX prototype that includes all unit operations expected in an industrial production plant, to validate this study. Such a scale up could be used as the basis for a more reliable application of LCA.

Acronyms and abbreviations

AL	Active layer
Bq	Becquerel
CFC-11	Trichloro(fluoro)methane
CHP	Combined heat and power
CPC	Compound parabolic collector
CCU	Carbon capture and utilization
DSP	Downstream processing
EPFL	École Polytechnique Fédérale de Lausanne
EPS	Expanded polystyrene
EU	European Union
FTO	Fluorine-doped tin oxide
GIS	Geographic information system
GJ	Gigajoule
GLO	Global
GWP100	Global warming potential for a time horizon of 100 years
ICFO	Photonic Science Institute
ICIQ	Catalan Institute for Chemical Research
IEM	Ion exchange membrane
ILCD	International Reference Life Cycle Data System
IPCC	Intergovernmental Panel on Climate Change
ISO	International organization for standardization
KBq	Kilobecquerel
kWh	Kilowatt-hour
LCA	Life cycle assessment
LCD	liquid crystal display
LCI	Life cycle inventory
LICROX	Light assisted solar fuel production by artificial CO2 reduction and water Oxidation
LPG	Liquefied petroleum gas
MJ	Megajoule
MEA	Monoethanolamine
nm	Nanometre
NPP_0	Net primary productivity
OPV	Organic photovoltaics
OCAP	Organic Carbon dioxide for Assimilation of Plants
P3HT	Poly(3-hexylthiophene)
PDF	Potentially disappeared fraction
PEC	Photoelectrochemical cell
PET	Polyethylene terephthalate
$PM_{2.5}$	Particulate matter 2.5 micrometres or less in diameter
PM6	Poly[(2,6-(4,8-bis(5-(2-ethylhexyl-3-fluoro)thiophen-2-yl)-benzo[1,2-b:4,5-b’]dithiophene))-alt-(5,5-(1’,3’-di-2-thienyl-5’,7’-bis(2-ethylhexyl)benzo[1’,2’-c:4’,5’-c’]dithiophene-4,8-dione)]
ppm	Parts per million

PVC	Polyvinylchloride
RER	Europe
RoW	Rest of the World
SCR	Selective catalytic reduction
TEG	Triethylene glycol
tkm	Tonne-km
TRTC	Two-Resonance Tapping Cavity
TUM	Technical University of Munich
UES	Unprotected ecosystem
Y6	2,2'-[[12,13-Bis(2-ethylhexyl)-12,13-dihydro-3,9-diundecylbisthieno[2'',3'':4',5']thieno[2',3':4,5]pyrrolo[3,2-e:2',3'-g][2,1,3]benzothiadiazole-2,10-diyl]bis[methylidyne(5,6-difluoro-3-oxo-1H-indene-2,1(3H)-diylidene)]]bis[propanedinitrile]

1 Introduction

1.1 The LICROX project

LICROX is a Research and Innovation Action project funded by the European Commission under the Horizon 2020 programme. The acronym LICROX stands for ‘Light assisted solar fuel production by artificial CO_2 reduction and water Oxidation’. The aim of the project is to produce and test a photoelectrochemical cell (PEC) for converting sunlight into organic molecules containing one or two carbon atoms, capable of storing chemical energy. Such organic molecules can then be used either as fuels or as platform chemicals.

A PEC can be understood as an artificial photosynthesis device which converts sunlight, water and carbon dioxide (CO_2) into carbon-based molecules, thus mimicking the natural process performed by plants in nature.

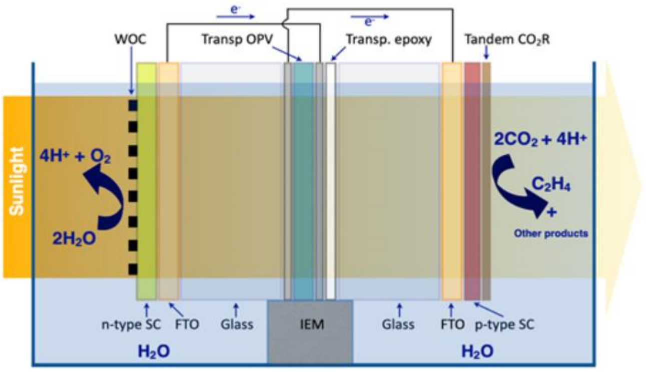

Figure 1. Schematic representation of the complete PEC configuration.

Figure 1 shows a schematic representation of the PEC under development by LICROX. The device consists of the main following components:

- A photoanode incorporating the water oxidation catalysts and light scattering elements.
- A semi-transparent organic photovoltaic solar cell (OPV).
- A nanostructured photocathode coupled to tandem catalysts for CO_2 reduction.

The two half cells are connected with electrical conductors and the anolyte and catholyte are separated with a suitable ion exchange membrane (IEM).

The LICROX project is coordinated by the Catalan Institute for Chemical Research (ICIQ) and counts with six other members in the consortium: The Technical University of Munich (TUM), the Photonic Science Institute (ICFO), the École Polytechnique Fédérale de Lausanne (EPFL), The Danish Board of Technology Foundation, and the companies Avantama and Hysytech. The project runs from September 2020 to August 2023 and it is expected to deliver a PEC prototype by the end of the project, to be built and demonstrated in the premises of Hysytech in Northern Italy.

More information about the project is available in the website: https://licrox.eu/

1.2 Life cycle assessment of LICROX

The LCA of LICROX is planned as a project including two stages or iterations:

- The first iteration, in which the study was conducted based on the data available by the consortium by the beginning of 2022. This iteration produced a first report, with a set of results communicated to the consortium in May 2022 and submitted for critical review.
- The second iteration, reported in the present document, as a result of a second round of data collection and refinement of the life-cycle model. Preliminary results from this second iteration have been communicated to the consortium and other stakeholders (researchers, industry, policymakers, environmental NGOs) in a workshop held in Copenhagen in September 2022. The present report has been submitted for critical review, with the final critically-reviewed LCA report expected by January 2023.

A key aspect of the LCA study is that it addresses a technology that is still under development. As a consequence, data collection constitutes a challenge, since the industrial activities delivering the targeted technology do not yet exist. The PEC prototype planned by the LICROX project is still under development too, and therefore many aspects that an LCA needs quantifying are yet to be defined. As a consequence, this kind of prospective assessments are subject to substantial uncertainty. On the one hand, sticking to real data provided by the consortium, often reflecting lab-scale conditions, leads to sub-optimal representation of production processes. On the other hand, portraying a full-scale deployment of this technology is not feasible, due to the large number of still undefined aspects. Thus, the approach we have taken is to, whenever possible, assess processes at industrial scale, even if on a theoretical basis or by taking similar technologies as an approximation. However, this has not been possible in all cases, and lab-scale data or small-scale production data needed to be used. This in contrast to the incumbent technology, steam cracking, a well-established and mature technology to produce olefins, for which ‘off-the-shelf’ inventory data can be obtained from most LCA databases or literature.

For these reasons, the results of this LCA should not be used to decide on whether or not the LICROX concept should be further pursued or otherwise scrapped. Instead, they can be used as an early indication of where this technology lies from an environmental standpoint, and to identify which key aspects would be most effective to focus on in order to improve its environmental performance.

1.3 About this report

This report describes the second and final iteration of the LCA study, following the ISO standards on LCA: ISO 14040:2006 and ISO 14044:2006. The report has been submitted for a critical review by an external LCA expert (see section 2.12).

2 Goal and scope definition

This section documents the first phase of the life cycle assessment (LCA), including a description of the purpose of the study, definition of the functional unit, an overview of the applied methods and an overview of the relevant processes (system boundary). This also includes important methodological choices affecting the other phases of the LCA study.

2.1 Standards

The study is carried considering the ISO standards on LCA: ISO 14040:2006 and ISO 14044:2006 as methodological guidelines. A critical review according to ISO/TS 14071: 2014 is performed by a single independent expert (see section 2.12).

2.2 Goal of the study

The goals of this study are twofold:

- To assess the life-cycle impacts of the LICROX technology at an early stage of development, in order to identify key hotspots and suggest potential improvement options.
- To compare LICROX with a conventional technology to produce ethylene, namely petrochemical steam cracking.

2.3 Intended application and audience

The LICROX consortium has commissioned the study in order to identify potential environmental improvement strategies in relation to the design of the PEC device and provide decision support both politically and in industries. Preliminary results have been communicated to selected stakeholders from academia, industry, policymakers and environmental NGOs in a workshop held by the consortium in Copenhagen by the end of September 2022. The communication/dissemination strategy to be followed after the study is completed remains to be decided by the consortium.

2.4 Product and systems under study

2.4.1 Ethylene

The target product for the two production processes under study is ethylene, a hydrocarbon with the formula C_2H_4. It is a flammable gas and the simplest alkene (a hydrocarbon with double carbon-carbon bonds). Globally, 183 million tonnes of ethylene were produced in 2019 (GPCA 2019), which exceeds the production volume of any other organic compound (Noah Chemicals 2021). The ethylene market is highly focused and concentrated on the production of polyethylene, due to the growing demand from various end-use industries such as construction, automotive and packaging, among others (CISION 2022). The most common industrial process for production of ethylene is via steam cracking of crude oil-based feedstocks (see section 2.4.2).

2.4.2 Production of ethylene by steam cracking

Thermal cracking, or steam cracking, is a petrochemical process in which saturated hydrocarbons are broken down into smaller, often unsaturated, hydrocarbons. It is the principal industrial method for producing the lighter alkenes (or commonly olefins), including ethylene and propylene. Steam cracker units are facilities in which a feedstock such as naphtha, liquefied petroleum gas (LPG), ethane, propane or butane is thermally cracked through the use of steam in steam cracking furnaces to produce lighter hydrocarbons.

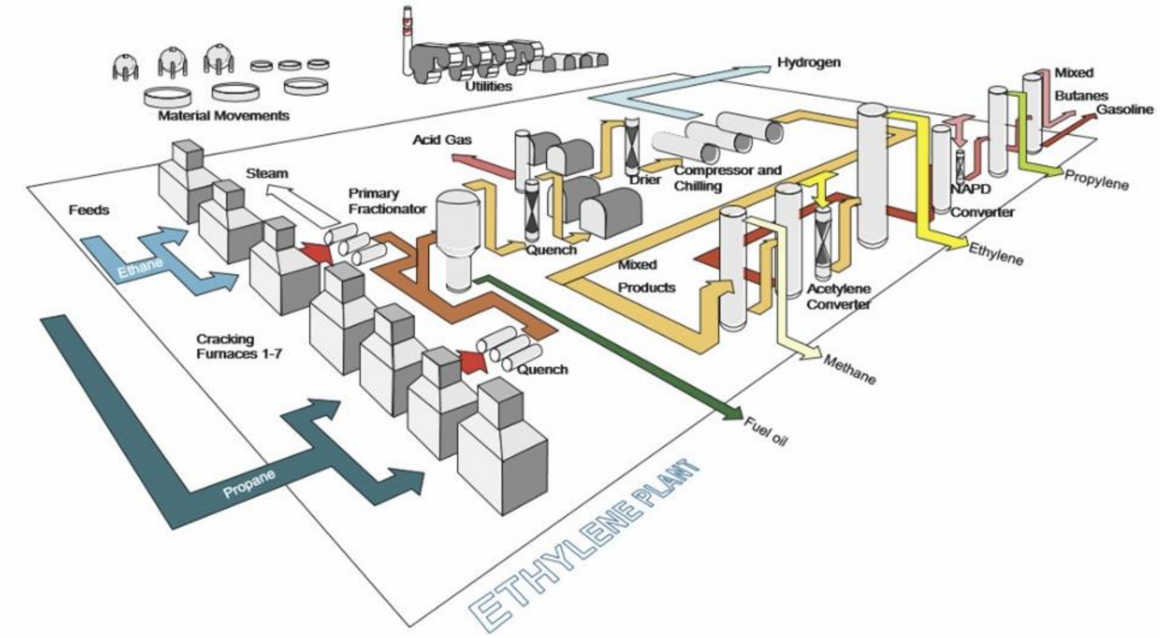

Figure 2. Overview of an ethylene production plant. Adapted from Buffenoir (2007).

According to Franklin Associates (2020) typical production begins when hydrocarbons are fed to the cracking furnace. After being pre-heated by a heat exchanger, mixed with steam and then further heated, the hydrocarbon feed is transferred to a reactor. The temperature is again increased to around 800 Celsius, and the cracked gas products are immediately cooled in quench towers using quench oil or quench water. Fuel oil is separated from the main gas stream in a multi-stage centrifugal compressor. The main gas stream then undergoes acid gas removal and drying to remove any moisture that may remain from the quenching process prior to cracked gas compression. The final step involves fractional distillation of the various reaction products and is achieved using a series of distillation columns and hydrogenation reactors. Within the hydrocracker, an off-gas is produced from the raw materials. A portion of this off-gas is processed and used as fuel gas to produce steam for the hydrocracker, while the remaining portion is exported from the hydrocracker as a co-product.

The main product from steam crackers is ethylene, but other valuable co-products are produced, such as propylene, C4 hydrocarbons such as butadiene, and pyrolysis gasoline, for example.

2.4.3 Production of ethylene by LICROX

Production of ethylene by means of the LICROX concept is assessed considering a hypothetical industrial plant, with an unspecified production capacity, located in Europe. This plant includes the following elements:

- The PEC device, installed in a ground installation, in a similar fashion as in a photovoltaic plant.
- Structural support and piping.

- An ultrapure water production unit.
- A chemical dosing station, from which CO_2 and electrolyte (potassium bicarbonate solution) are supplied.
- Auxiliary devices such as pumps, control and monitoring system, sampling and gas analysis system.
- A downstream processing unit (DSP), which will mainly consist of a gas separation process by means of pressure swing adsorption (PSA).

Overall, the chemical reaction occurring in the PEC can be summarized stoichiometrically as:

$$2CO_2 + 2H_2O \rightarrow C_2H_4 + 3O_2$$

Equation 1. Chemical reaction for production of ethylene in the PEC.

The main raw material for this production process is CO_2 as carbon source. In an industrial-scale scenario, the LICROX plant is assumed to be located in the vicinity of industrial activities where CO_2 is obtained as a by-product, compressed and transported via pipeline to the LICROX plant, instead of being liquified and transported by tanker/truck, which is more costly. As an example of such a carbon capture and utilization (CCU) scheme, the network of pipelines operated by OCAP (Organic Carbon dioxide for Assimilation of Plants), a subsidiary of Linde gas, supplying CO_2 to horticultural greenhouses in the Rotterdam area, is taken. In an alternative scenario, on request by the consortium, the study considers the direct use of unprocessed flue gases from a nearby power plant, also transported via pipeline to the LICROX plant.

The electron donor for the chemical reaction in the PEC device is water. For this, ultrapure water will be supplied from an on-site production unit. Within a PEC, water is oxidized in the photoanode, producing oxygen. In the photocathode, CO_2 is reduced to ethylene. The electrolyte used in the PEC is a solution of potassium bicarbonate, that needs to be replaced periodically. The produced ethylene is subject to a separation and purification process in the DSP unit, where it is separated from excess CO_2, the produced oxygen, etc. in a pressure swing adsorption unit. CO_2 is recirculated, while other gases are ultimately vented to the atmosphere. Ethylene is finally pressurized and stored.

2.5 Function and functional unit

Both assessed systems have the production of ethylene as main function. Any additional functions, such as the production of other useful materials or fuels are dealt with by means of system expansion (substitution), in such a way that in both systems the only remaining function is ethylene production. The functional unit and reference flow used in the study is 1 kg ethylene.

2.6 Life cycle inventory modelling approach

The results of the present study are calculated according to consequential standards/methods for LCA in accordance with the specifications of the international standards for LCA: ISO 14040:2006 and 14044:2006. In particular, co-production is handled by means of substitution in compliance with Step 1 of the allocation procedure in section 4.3.4.2 of ISO 14044:2006. The applied methodology is further defined in Weidema et al. (2009).

Consequential modelling is a cause-effect based approach to the definition of system boundaries in LCA (Sonnemann and Vigon, 2011), and it is characterized by the modelling of by-products using substitution and by including only unconstrained suppliers in the market mixes. The results of a consequential model can be interpreted as the expected impacts induced by a demand for the reference flow.

Consequential LCA gives an answer on the question: "*what is the impact of a choice?*" This choice could be to buy or produce a product (compared to not buy or produce the product), or to implement an improvement option. Consequential LCA is relevant when companies/decision makers want to know the impacts of their actions.

2.7 Product system and system boundaries

2.7.1 Product system

The study can be considered as a 'cradle-to-gate' LCA of ethylene, since the downstream stages of ethylene conversion to final products, their use and disposal are excluded. This is justified given that they are expected to be the same regardless of how the ethylene is produced, and therefore they become irrelevant from a comparative point of view. Regarding the LICROX plant as such, the study can be considered as a 'cradle-to-grave' one, since we are addressing the production, use and decommissioning of a hypothetical industrial plant.

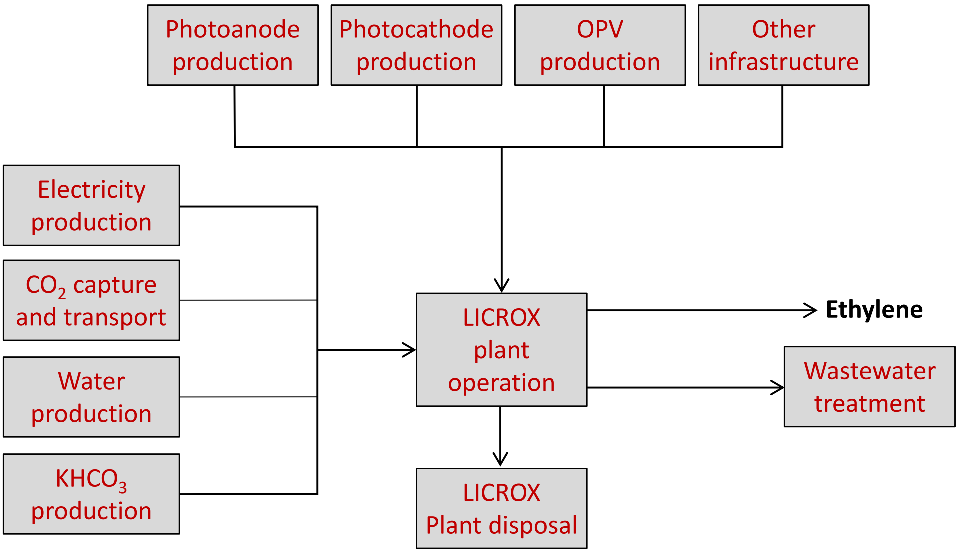

Figure 3. Foreground system for the life cycle of ethylene production by the LICROX concept. $KHCO_3$: potassium bicarbonate.

Figure 3 shows a diagram for the foreground system of the LICROX plant. It includes the production of the plant infrastructure, namely PEC components (photoelectrode, OPV) as well as other infrastructure (structures, piping, etc.) and its disposal at the end of its useful life. Plant operation requires inputs of grid electricity, chemicals (carbon dioxide and potassium bicarbonate) and water. The relevant outputs from the plant operation are ethylene, the spent electrolyte solution, which is discharged as wastewater, and emissions of by-product gases (not shown in the figure). PEC and other plant infrastructure disposal leads to the generation of solid waste and scrap (not shown in the figure), part of which is expected to be ultimately recycled, such as metal scrap and glass. Other materials, most notably plastic, are expected to be landfilled or incinerated, the latter leading to recovery of energy.

Figure 4 shows the equivalent diagram for ethylene production by steam cracking, based on data from Rodríguez-Vallejo et al. (2020). The main inputs to the production process are naphtha, used as feedstock, energy carriers, as well as plant infrastructure. It can be seen that the process produces several by-products, namely propylene, hydrogen, and C4 and C5 hydrocarbons. C4 hydrocarbons are assimilated to butadiene, as this is the most abundant C4 hydrocarbon from steam crackers (Jukić 2013), while the C5 Hydrocarbon fraction is assimilated to pyrolysis gasoline, the other main by-product from steam crackers (Jukić 2013). Co-production is included in the model as a substitution of equivalent amounts of materials from the corresponding marginal suppliers.

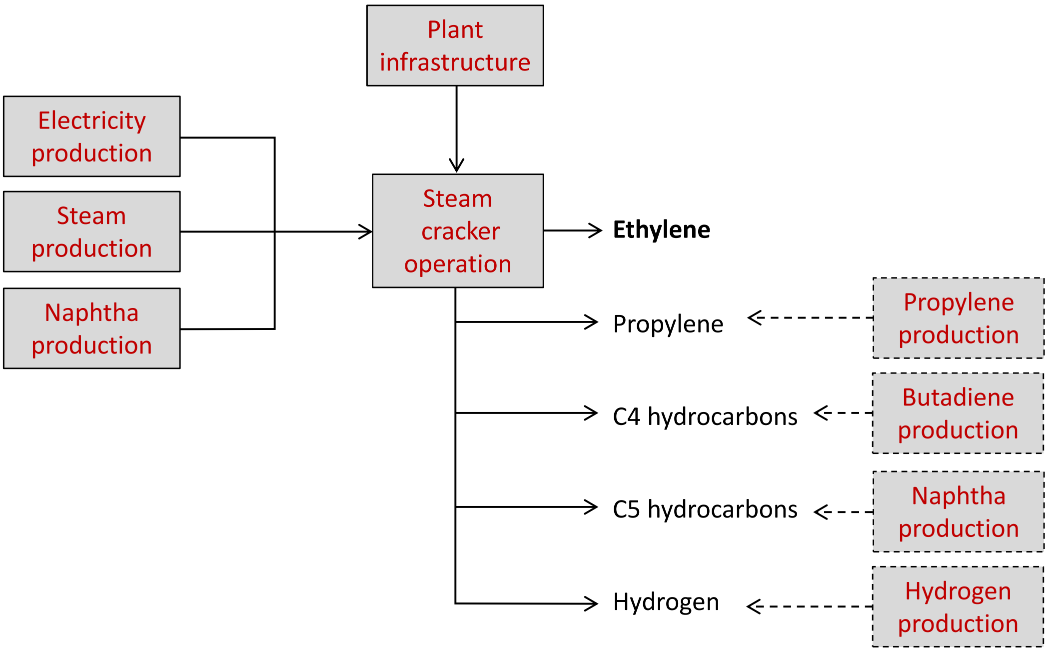

Figure 4. Foreground system for the life cycle of ethylene production by steam cracking. Dashed-line box indicates a substitution.

2.7.2 Geographic and time delimitation

The geographic focus of this study is Europe, as the LICROX project is an EU-funded project. Production of the PEC device is considered in the study to take place in Europe, while for the supply of the underlying materials an average global scenario is considered in the inventory analysis. The reason for this is that many of these materials, such as chemical precursors, etc., are expected to be traded in the global market. As a consequence, ideally a global marginal supply mix should be used. In practice, though, defining marginal supply mixes for a plethora of chemicals is not feasible given the time and resources available for this study. A global average approach is deemed as the second-best approach available.

For ethylene produced by steam cracking, the affected supply is also considered to be Europe. In this way, it is assumed that a demand for ethylene from steam cracking is not supplied from a global market, but from a local market. According to IEA (2018), trade in primary chemicals tends to be modest relative to that of the downstream derivatives, mainly because of high transportation costs and low margins. The local market for petrochemical ethylene in this study is modelled as Europe.

Regarding time delimitation, the model includes activities which are expected to take place at different points in time, such as the production of the LICROX plant components and the dismantling of this plant. In the study all activities are modelled as happening in the same year. In other words, there is no discounting, or otherwise, of environmental impacts taking place in the future.

2.7.3 Cut-offs

In the foreground system for the LICROX model no deliberate cut-offs have been applied. Whenever a known activity is excluded, this is due to lack of data. An effort has been made to include all possible activities, even if done with rather uncertain data. Regarding ethylene from steam cracking, no cut-offs have been applied either, and all foreground data in the original source (Rodríguez-Vallejo et al. 2020) are used.

In the background system, the ecoinvent database is used (see section 2.8.3). This database does include infrastructure, but it systematically omits inputs of services (Font-Vivanco 2020).

2.8 Data sources and quality

Data used in the study are distinguished at two levels: foreground data, referring to the activities displayed in the life cycle diagrams (Figure 3, Figure 4) and background data, referring to the data obtained from the ecoinvent database.

2.8.1 Foreground data: ethylene production by LICROX

A detailed account of the quality of each single data point supplied by the LICROX consortium or chosen by 2.-0 LCA consultants is not feasible, given the complexity of the developed model. We provide instead here a qualitative description of the data used. A detailed description of the data used is provided in chapter 3.

Foreground data used to build the life-cycle of the LICROX technology are described in the paragraphs below for four separate groups of activities:

- Production of the PEC and its components.
- LICROX plant infrastructure.
- LICROX plant, PEC operation.
- LICROX plant, DSP operation.
- LICROX plant dismantling.

Production of the PEC device and its underlying components constitutes by far the most complex part of the LICROX life cycle inventory, given the large number of components involved. The LICROX consortium has provided data on the specific materials, or otherwise their chemical precursors, incorporated in the device, per m^2 PEC. Whenever possible, such materials have been covered by ecoinvent data sets, as for example in the case of glass or PET, but in many cases specific inventories have been developed, as in the case of nanomaterials, for example. Such specific inventories have been built either based on literature data describing the same or similar process (see copper nanoparticles, for example), or based on stoichiometry and taking data on utilities (energy, water use, etc.) from similar processes in the ecoinvent database (see bismuth nitrate, for example). Whenever data on a chemical production process have been provided by the consortium, this typically reflects lab-scale or small production volumes, and the data are often incomplete. In spite of this, these data have been used whenever industrial-scale production data were not available. Finally, data on manufacturing the PEC (sputtering, roll-to-roll processing, thermal evaporation, gravure coating, encapsulation) have been compiled by ICFO to reflect a real industrial process, even if hypothetical.

Data on the infrastructure needed to build a full-scale LICROX plant were simply not available at this stage of the LICROX project, where even the prototype design is not ready. This means the project cannot feed any data to the LCA regarding such elements as structural parts, piping, pumps, tanks, land requirements, PSA unit, etc. Omitting these aspects in the study would constitute an important gap and for this reason our approach has been to try and approximate these infrastructure requirements with the closest data source available. Potential sources of data for this would be, for instance, LCA studies of photovoltaic plants, but they have been judged not to properly represent a chemical production facility as the one LICROX is targeting. Another potentially useful source is the LCA for a PEC-based plant producing hydrogen, as described by Sathre et al. (2014), however the inventory data are not reported in sufficient detail to be able to reproduce them to a satisfactory level. In the end, we have opted to represent the LICROX infrastructure with data describing a solar-assisted photocatalysis plant treating industrial wastewaters in Spain, as reported by Muñoz (2006). With these data we attempt to cover the requirements for civil engineering, structural materials, piping, etc., excluding the equipment for ultrapure water production, or downstream processing of the produced gases. Ultrapure water production equipment is implicitly covered by the ecoinvent data set used for this activity (see paragraph below), which does account for infrastructure (reverse osmosis modules, etc.). Regarding DSP, infrastructure is approximated by means of a detailed bill of materials for an industrial pressure swing adsorption unit for purification of biogas, as described by Kohlheb et al. (2021).

Data on operation of a hypothetical LICROX plant were equally scarce. The main mass balance for the production process has been based on the stoichiometry shown in Equation 1, assuming the overall efficiency in the use of CO_2 is 80%. The inventory for CO_2 capture, pressurization and transport via pipeline is based on literature (Rosental et al. 2020; Croezen et al. 2018) as well as published data by the OCAP grid (OCAP 2018). The inventory for unprocessed flue gas supply via pipeline has been built using data and assumptions from studies on microalgae cultivation using such flue gases (Brentner et al. 2011; Campbell et al. 2011). Several key aspects required in the inventory were suggested by the consortium as a best guess at this early stage of technology development, namely the aforementioned CO_2 utilization efficiency, PEC useful life (established in 10 years as a desirable target), the ethylene yield (set at 0.015 kg/m^2 PEC-day), the composition and replacement rate for the electrolyte, and the electricity consumption by the plant. Ultrapure water production is covered by the ecoinvent database, which is judged to properly represent average equipment and operation requirements for this activity. Finally, data on the treatment of the spent electrolyte as wastewater are considered to be complete and representative of European conditions. The inventory for this activity has been obtained with the WW LCI model developed by 2.-0 LCA consultants (Muñoz 2021).

Finally, the end-of-life stage for the LICROX plant has been established based on the material characterization of the PEC and other plant infrastructure and assuming a plausible fate for each material, chiefly recycling/disposal. In general, metals in big structural elements or machinery have been assumed to be recycled, while plastics and inert materials are assumed to be sent for disposal. In the particular case of the PEC, it is assumed that the glass sheet can be recycled, while the remaining materials are disposed of. The inventory includes the transport and treatment of each material as waste, as well as any substitution of primary raw materials or energy, as a result of recycling and incineration with energy recovery. The plant dismantling operation as such is not included.

2.8.2 Foreground data: ethylene production by steam cracking

Ethylene is a basic building block for the petrochemical industry, and as such it is typically included in LCA databases. However, to our knowledge, a consequential life cycle inventory of the steam cracking process to produce ethylene does not exist.

The ecoinvent database v3.6 is the first place to look for such data, as it is the background database used in this study. The database includes average data for ethylene production in Europe, where the primary data source is the European plastics industry (PlasticsEurope) and the data seems to be as old as from 1999. An additional limitation of this data set is the fact that it comes in an aggregated form, where only elementary flows are reported. This is a limitation as this data format does not allow for modifications or updates of the data set to try and reflect changes in production methods (changes in raw materials used, mass balances, etc.). For these reasons a decision has been made not to use this data set.

PlasticsEurope (2012) also provides inventory data for average ethylene production in Europe in 2008-2010, however it presents the same limitations described above for the ecoinvent data set, and for this reason their use has also been discarded.

Similarly, the US LCI database (NREL 2022) provides a data set for ethylene production, produced by Franklin Associates (2020). The data set describes production of ethylene in the United States and Canada, with data directly obtained from producers reflecting production in 2015. The individual data from producers was then used to obtain a weighted average according to production volumes of each producer. The methods used to build the model deviate from those targeted in the present study, with some deliberate cut-offs and given that co-production in the steam cracker is handled by means of mass allocation (the same approach used by PlasticsEurope). For this reason, this data set has also been finally discarded.

As a result of this literature search, we realized that the present study would need to resort to developing a dedicated model for ethylene production from steam cracking. This requires, in addition, to develop a model for production of propylene, the main by-product from steam cracking. Both models have been built based on primary data by Rodríguez-Vallejo et al. (2020), providing a sufficiently detailed mass and energy balance for steam cracking using naphtha as feedstock, and for propylene production using methanol as feedstock, the latter identified as the marginal production technology in Europe (see section 3.6.2). The mass and energy balances provided by Rodríguez-Vallejo et al. (2020) for steam cracking were sourced from the work of Yang and You (2017), while the data for propylene production from methanol were elaborated by the authors themselves. In both cases, though, the data were obtained as a result of process simulation using the Aspen HYSYS software. The authors applied economic allocation in order to deal with the joint production processes of steam cracking and methanol-to-propylene, however the data are reported before allocation, and this is the format that has been used in order to build a consequential model in the present study.

2.8.3 Background data: ecoinvent

The background system is modelled with the ecoinvent database, version 3.6, specifically the ‘Substitution, consequential, long-term’ system model. This is consistent with the life cycle inventory (LCI) modelling approach established in section 2.6, as this system model uses substitution to solve multifunctionality issues and includes only unconstrained suppliers in the market mixes.

2.9 Impact assessment methods

The method used for impact assessment is ‘Stepwise’. The method is described and documented in Annex II in Weidema et al. (2008) and in Weidema (2009). This method was developed by 2.-0 LCA consultants choosing the best principles from the Danish EDIP 2003 method (Hauschild and Potting 2005) and from the Impact 2002+ method (Jolliet et al. 2003). In total, Stepwise includes a total of 16 impact categories, as shown in Table 1.

Stepwise has the option of presenting results at two levels:

- Characterization, also called midpoint, where each impact category is presented individually, with its own units, as shown in in Table 1.
- Endpoint, where each impact category is expressed in a common unit expressing damage. In Stepwise, damage is expressed in monetary units, namely EUR_{2003}.

Endpoint modelling through monetarisation using the budget constraint concept (see Weidema 2009) is a unique feature of Stepwise and the main reason for choosing this method.

Table 1. Impact categories included in the study.

Impact category	Unit	Description
Acidification	m^2 UES	The unit expresses the area of ecosystem within the full deposition area (in Europe), which is brought to exceed the critical load of acidification as a consequence of the emission (area of unprotected ecosystem = m^2 UES). The impact indicator is based on modelling of deposition in Europe. (Hauschild and Potting 2005, p. 47)
Ecotoxicity, freshwater	kg TEG-eq into water	Impact on freshwater ecosystems from chemicals released into the environment is expressed in kg triethylene glycol (TEG) emitted to water. The model considers fate, exposure and effects of organic and inorganic (metals) chemicals, using the IMPACT 2002 model (Pennington et al. 2005, 2006).
Ecotoxicity, terrestrial	kg TEG-eq into soil	Impact on terrestrial ecosystems from chemicals released into the environment is expressed in kg triethylene glycol (TEG) emitted to soil. The model considers fate, exposure and effects of organic and inorganic (metals) chemicals, using the IMPACT 2002 model (Pennington et al. 2005, 2006). The model assumes that ecotoxic effects occur only by exposure through the aqueous phase in soil.
Eutrophication, aquatic	kg NO_3-eq	The aquatic eutrophication potentials of a nutrient emission express the maximum exposure of aquatic systems that it can cause. The aquatic eutrophication potentials are expressed as N- or P-equivalents. (Hauschild and Potting 2005, p. 73-74)
Eutrophication, terrestrial	m^2 UES	The unit expresses the area of ecosystem within the full deposition area (in Europe), which is brought to exceed the critical load of eutrophication as a consequence of the emission (area of unprotected ecosystem = m^2 UES). The impact indicator is based on modelling of deposition in Europe. (Hauschild and Potting 2005, p. 47)
Global warming	kg CO_2-eq	The unit is global warming potential for a time horizon of 100 years (GWP100) (kg CO_2 equivalents) based on the IPCC fifth assessment report (Myhre et al. 2013) adapted as described by Muñoz and Schmidt (2016). CO_2 emissions from biogenic sources do not contribute to global warming, except if arising from land use changes
Human toxicity, carcinogens	kg C_2H_3Cl into air	Impact on human health related to emissions of chemicals is expressed in kg chloroethylene into air. The model considers fate, exposure and effects of chemicals using the IMPACT 2002 model (Pennington et al. 2005, 2006). Characterization factors are applied to carcinogenic substances only.
Human toxicity, non-carcinogens	kg C_2H_3Cl into air	Impact on human health related to emissions of chemicals is expressed in kg chloroethylene into air. The model considers fate, exposure and effects of chemicals using the IMPACT 2002 model (Pennington et al. 2005, 2006). Characterization factors are applied to non-carcinogenic substances only.
Mineral extraction	MJ extra	Expected increase in extraction energy per kg extracted material. The reasoning is based on the fact that extraction of minerals exploits the ores with the highest concentrates (most accessible) resources first. (Goedkoop and Spriensma 2001, p 14)
Nature occupation	PDF·m^2·yr	Represents the impact from the occupation of one m^2 of land during one year, where the impact is assessed on the basis of the duration of area occupied (m^2·years) multiplied with a severity score, representing the potentially disappeared fraction (PDF) of species on that area during the specified time (Schmidt and De Saxcé 2016)
Non-renewable energy demand	MJ primary	Total use of primary non-renewable energy resources (coal, oil, natural gas) measured in MJ.
Photochemical ozone, vegetation	m^2·ppm·h	The impact is expressed as the accumulated exposure (duration times exceedance of threshold) above the threshold of 40 ppb times the area that is exposed as a consequence of the emission. The threshold of 40 ppb is chosen as an exposure level below which no or only small effects occur. The unit for vegetation exposure is m^2*ppm*hours. (Hauschild and Potting 2005, p 93)
Respiratory inorganics	kg $PM_{2.5}$-eq	The impact on human health related to respiratory inorganics is expressed as equivalents of particles ($PM_{2.5}$).
Respiratory organics	Person·ppm·h	Covers the impact on human health from photochemical ozone formation. The impact is expressed as the accumulated exposure above the threshold of 60 ppb times the number of persons exposed as a consequence of the emission. The unit for human exposure is person*ppm*hours. (Hauschild and Potting 2005, p 93)
Ionizing radiation	Bq Carbon-14 into air	Damage to human health from exposure to radioactive isotopes. Based on the Ecoindicator 99 method (Goedkoop and Spriensma 2001). Includes substances classified in IARC groups 1, 2A, 2B and 3 for which sufficient information on physico-chemical characteristics and carcinogenesis is available. Fate of substances is calculated with the EUSES model, and effects are based on probability of cancer.
Ozone layer depletion	kg CFC11-eq	Impact on the ozone layer is expressed in kg CFC-11 into air-eq, obtained from the US Environmental Protection Agency Ozone Depletion Potential List.

2.10 Additional methodological aspects

2.10.1 Carbon accounting

In this study, CO_2 emissions from biogenic sources do not contribute to global warming, except if arising from land use changes (see section 2.10.2). Also, an important aspect in this study is that we are comparing petrochemical ethylene, incorporating carbon from fossil origin, with ethylene that uses industrial CO_2 as carbon source. The question is how to consider these differences in the study.

First of all, industrially-supplied CO_2 is a by-product of industrial processes such as ammonia and hydrogen production (Pierantozzi 2003). Its use as a reagent by the LICROX plant simply avoids its venting to the atmosphere. As a consequence, when CO_2 is used in the LICROX plant, the net effect is a delay in the CO_2 emission, which will now take place at the end-of-life stage of ethylene-based products, instead of during e.g. fertiliser manufacturing. In this way, the demand for this CO_2 reagent has no net effect on global warming, if the effect of this delay is neglected. Thus, we treat this CO_2 in the study in the same way as biogenic CO_2. This is in contrast to the CO_2 from an eventual degradation/combustion of petrochemical ethylene, which is certainly from fossil origin and has a contribution to global warming.

A second point to bear in mind is that this LCA study has cradle-to-gate boundaries, while the carbon embedded in ethylene will only be released to the atmosphere at the end-of-life stage, which is excluded from the study. In order to have a meaningful account of the different carbon source in the two ethylene production routes, in this study we apply a CO_2 credit (an emission of negative sign) to ethylene from the LICROX plant, calculated as -1 kg CO_2 per kg CO_2 supplied to the plant. This can be understood as the amount of CO_2 that LICROX ethylene has temporarily sequestered from the atmosphere, as opposed to petrochemical ethylene which does not achieve such sequestration. It could be argued that ethylene derivatives such as polyethylene, if sent to a landfill, will not degrade at all, and that therefore in such a scenario it does not matter if the carbon in ethylene was biogenic or fossil, and that this invalidates our credit. This is in fact not the case, since landfilling of LICROX ethylene does achieve a carbon sink (it contains carbon that would have otherwise been emitted to the atmosphere), while petrochemical ethylene does not achieve a carbon sink (its carbon comes from oil and gas reserves in the ground, and this carbon ultimately returns to the ground, but no carbon from the atmosphere is sequestered).

2.10.2 Indirect land use change

In this study we address land use change effects by means of the model developed by Schmidt et al. (2015) for so-called ‘indirect land use change’ (iLUC). As a default, industrial activities such as the LICROX plant or a steam cracker are assumed to demand land that was previously used for agriculture, as this is typically flat, easily accessible land. As an example, evidence for this pattern is provided by Zhang et al. (2021), showing that in China, between 1990 and 2015, industrialization has led to the loss of 1.76 million hectares of cropland, implying a loss in crop production of 6.49 million tonnes per year.

In this way, the agricultural activity is displaced by the industrial activity and it needs to be carried out somewhere else, since the demand for its agricultural products remains unchanged. According to the model by Schmidt et al. (2015), this compensation for the lost agricultural production occurs partly as expansion of arable land (deforestation), and partly as intensification of agricultural land already in use. The environmental effects of this compensation are what we call iLUC. The model by Schmidt et al. (2015) assumes that there is a global market for land. To be more precise, the market is not mainly concerned with the area of land but rather with its production capacity. Hence, all countries that expand their arable land supply production capacity into this market, while all countries that intensify their existing agricultural land also supply production capacity into this global market.

We consider iLUC effects only for the ethylene production plants, for both the LICROX technology and steam cracking. The quantification of iLUC effects for a given activity (further described in section 3.2.3), requires determining two basic variables: the amount of land occupation, and the productivity of this land, measured as its potential primary production (NPP_0) in g carbon/m^2-year.

2.11 Software

The life-cycle model is implemented in the LCA software SimaPro 9.1.1.1 (Pré Sustainability 2021).

2.12 Critical review

This LCA study is subject to a critical review according to ISO/TS 14071: 2014, performed by a single independent external expert, Dr. Miguel Brandão, Associate Professor in Industrial Ecology and Life Cycle Assessment at KTH, Stockholm. The review report is available in the Appendix.

3 Life cycle inventory analysis

The purpose of the life cycle inventory (LCI) analysis is to quantify, in as much detail as possible, all the mass and energy flows in the system under study. Inventory data are structured in tables which may include the following items:

- Reference flow: the product or service obtained in the inventoried activity.
- By-products: secondary products or services obtained. They are shown with a negative sign, indicating that they substitute an equivalent amount of product or service.
- Inputs of natural resources: inputs of resources directly extracted from nature, such as water or land. Resources that have been subject to some transformation, such as tap water, are not included here but as an input of products and services (see bullet below).
- Inputs of products and services: details inputs from the economic system, such as raw materials, components, energy carriers, other services, etc.
- Emissions to air: direct emissions of pollutants by the inventoried process. These emissions are not related to the use of fuels, which are separately included in the data sets for inputs of energy carriers.
- Emissions to water: direct emissions of pollutants by the inventoried process, to such compartments as rivers, coastal waters, etc.
- Emissions to soil: direct emissions of pollutants by the inventoried process, to agricultural soil.

3.1 Photoelectrochemical cell manufacturing

The PEC device consists of two main functional parts:

- The photoelectrode, consisting of photoanode and photocathode.
- The organic photovoltaic system.

These two parts are ultimately assembled into a full PEC device. This section describes data used to derive the inventories for PEC manufacturing, such as amounts of components, auxiliary materials, energy use, etc. The overall inventory for PEC manufacturing, per m^2 device, is shown in section 3.1.5. For those individual activities that cannot be directly covered by existing data sets in the ecoinvent database, we provide specific inventories, in sections 3.1.6 to **Error! Reference source not found.**.

The inventory assumes that the manufacturing process takes place in an unspecified European country. This is included in the model as an average European production scenario.

3.1.1 Manufacturing: photoelectrode materials

A summary of the materials involved in photoelectrode manufacturing is given in Table 2, according to two photoanode material options. Further details on these data are provided in the paragraphs below.

Table 2. List of materials used in photoelectrode manufacturing, per m^2 PEC.

Exchange	Unit	PEC ($BiVO_4$)	PEC ($TiFe_2O_5$)	Comments
Glass substrate	kg	2.5	2.5	1 cm thickness.
FTO solution	L	0.131	0.131	For a 500 nm layer. Estimate based on Tsang (2016), reporting 0.042 L solution are needed for a 160 nm layer.
Bismuth nitrate	kg	0.025		$BiVO_4$ precursor for a 100 nm layer.
Vanadyl acetylacetonate	kg	0.002		$BiVO_4$ precursor for a 100 nm layer.
Acetylacetone	kg	0.49		$BiVO_4$ synthesis solvent.
Pseudobrookite nanoparticles dispersion	kg		0.01	100 nm layer obtained from a 2.5% by weight dispersion of pseudobrookite nanoparticles in isopropanol.
Copper nanoparticles	kg	0.002	0.002	Precursor for a 100 nm layer of $CuFeO_2$.
Iron oxides nanoparticles	kg	0.002	0.002	Precursor for a 100 nm layer of $CuFeO_2$.
Molecular catalyst	kg	0.003	0.003	Best estimate by ICIQ is 2.5 g/m^2.
Copper nanoparticles	kg	0.00015	0.00015	Best estimate by EPFL is 150 mg/m^2.

According to TUM, the photoelectrode includes a 1-cm thick glass substrate, a 500-nm thick fluorine-doped tin oxide (FTO) layer, a 100-nm Bismuth vanadate ($BiVO_4$) layer and a 100-nm thick delafossite ($CuFeO_2$) layer. According to Avantama, an alternative to $BiVO_4$ would be a layer of pseudobrookite ($TiFe_2O_5$) nanoparticles, of the same thickness.

In addition, according to ICIQ the photoelectrode requires 0.5 to 2.5 g/m^2 of a porphyrin-based molecular catalyst, plus a similar amount of another molecular catalyst with similar molecular structure. In the inventory, it is assumed that 1.5 g of each catalyst are needed per m^2 PEC. Finally, according to EPFL 150 mg/m^2 of copper nanoparticles are required.

Based on the thickness (1 cm) and density of glass (2.5 kg/L), the amount of glass can be calculated. In addition, TUM has provided the necessary amounts per m^2 of the different precursors to obtain the $BiVO_4$ and $CuFeO_2$ layers, namely bismuth nitrate, vanadyl acetylacetonate, acetyl acetone, copper nanoparticles and iron oxides nanoparticles. Inventories for all these materials have been produced for this study, as described in sections 3.1.6, 3.1.7, 3.1.8 and 3.1.9, with the exception of glass and acetylacetone, for which default data sets in the ecoinvent database are considered to be sufficient. Data on the FTO coating materials has been estimated based on data from Tsang (2016), who provides an inventory for producing this coating in an ethanol-water solution, reporting that 0.042 L of such a solution is needed per m^2 for a 160 nm layer. Here we assume that this dose increases in proportion to the thickness, whereby a 500-nm layer would require 0.131 L of solution. The inventory data for this solution are described in section 3.1.10.

The $BiVO_4$ (or alternatively $TiFe_2O_5$) and $CuFeO_2$ layers require an annealing process, for which an estimate of energy consumption is provided in section 3.1.3. Regarding the molecular catalyst, also a specific inventory has been developed for this study (section 3.1.11). Finally, the amount of pseudobrookite nanoparticles needed for a 100-nm thick layer is 10 g/m^2 of a dispersion of these particles in isopropanol, according to Avantama. A specific inventory for this dispersion is provided in section 3.1.12.

3.1.2 Manufacturing: Organic photovoltaic materials

The inventory of components in the OPV has been provided by ICFO, as a detailed bill of materials, where most of these are quantified based on the layer thickness and densities. The OPV is assumed to use a polyethylene terephthalate (PET) substrate. A summary of the materials involved is given in Table 3, per m^2 PEC, which equals 1 m^2 OPV. The amount of copper required for connecting the OPV to the photocathode and photoanode could not be quantified by ICFO and is therefore not included.

Most materials in Table 3 have been included in the model by means of existing data sets in the ecoinvent database, however specific inventories have been developed for production of zinc acetate dihydrate (section 3.1.13) and the active layer polymers PM6/Y6 (section 3.1.14).

Table 3. List of materials used in OPV manufacturing, per m^2 PEC.

Material	Unit	Amount	Comments
OPV materials			
PET substrate	kg	6.90E-02	50 µm thick PET film.
Light management 1 (SiO_2 target)	kg	1.06E-03	Light management to improve photoanode response. Constituted by 4 layers, 100 nm each, intercalating SiO_2/TiO_2 deposited by roll-to-roll (R2R) sputtering.
Light management 1 (TiO_2 target)	kg	1.69E-03	
TRTC 1 (zinc oxide target)	kg	2.81E-05	Two-Resonance Tapping Cavity (TRTC), 5 nm thick film deposited by R2R sputtering.
TRTC 2 (thin silver target)	kg	7.34E-05	7 nm thick film deposited by R2R sputtering.
TRTC 3 (zinc oxide target)	kg	2.81E-05	5 nm thick film deposited by R2R sputtering.
Zinc acetate dihydrate	kg	1.12E-04	20 nm thick film deposited by R2R Slot-die coating from a precursor solution, followed by drying at 150ºC.
2-methoxyethanol (zinc oxide solvent)	kg	3.53E-06	
Ethanolamine (zinc oxide additive)	kg	3.53E-08	
Active layer (AL) donor, PM6	kg	5.50E-05	100 nm thick film deposited by R2R Slot-die coating, followed by drying at 100ºC. The precursor solution is a 16 mg/ml chloroform mixture of polymer donor (PM6) and non-fullerene acceptor (Y6). The donor:acceptor ratio is 1:1.2 on a mass basis. The amounts of donor and acceptor polymers include an additional 10% mass, to account for edge effects. Chloronaphthalene constitutes 0.5% of total solution volume.
Active layer (AL) acceptor, Y6	kg	6.60E-05	
Chloroform (AL solvent)	kg	5.08E-06	
Chloronaphthalene (AL additive)	kg	3.17E-08	
Molybdenum trioxide	kg	2.35E-05	5 nm thick film deposited by R2R vacuum thermal evaporation.
Thin silver pellets	kg	9.44E-05	9 nm thick film deposited by R2R vacuum thermal evaporation.
Thick silver connect ink	kg	1.31E-02	25 µm thick edge electrode contacting the thin silver layer (5% of 1 m^2).
Light management 2 (Lithium fluoride)	kg	4.75E-04	2 layers (140 and 40 nm) of Lithium fluoride, intercalated by 1 layer of Molybdenum trioxide (100 nm) deposited by R2R vacuum thermal evaporation.
Light management 2 (Molybdenum trioxide)	kg	4.69E-04	
Copper interconnectors	kg	-	Interconnecting: 1) the OPV with the photoanode; 2) the OPV with the photocathode. Amount to be determined.
Encapsulation materials			
Adhesive epoxy	kg	2.93E-02	25 µm epoxy resin, UV curable, that bonds the bottom and top PET films and acts as encapsulant.
PET Barrier	kg	6.90E-02	50 µm thick PET film.

3.1.3 Manufacturing: processing of materials

On the one hand, production of the photoelectrode includes the FTO coating process as well as the annealing of the $BiVO_4$ (or alternatively $TiFe_2O_5$) layer and $CuFeO_2$ layer. On the other hand, OPV manufacturing involves a series of sputtering, roll-to-roll processing, thermal evaporation and gravure coating processes, as well as the final encapsulation of the PEC device.

From a material point of view, we include in the inventory the amount of argon gas required for the sputtering process, namely 603 L/m^2 PEC, or 1.08 kg/m^2, as estimated by ICFO. Other auxiliary materials, such as solvents, have been included as part of the materials listed in sections 3.1.1 and 3.1.2.

Regarding energy use, the entire process is considered to rely on electricity only, according to ICFO. A summary of the electricity consumption on a m^2 PEC basis and broken down by process is displayed in Table 4. Two cases are shown in the table, according to whether $BiVO_4$ or $TiFe_2O_5$ is used in the photoanode, given that the annealing temperature is different, 500 ºC and 750 ºC, respectively. Energy consumption for the annealing processes constitutes a crude estimate, based on the specific heat capacity of glass (constituting more than 99.5% of the substrate mass), the required temperature increase from 15 ºC and assuming the oven efficiency is 25% (Bureau of Energy Efficiency 2005). This estimate accounts for the energy required to heat the material to the desired temperature, but the energy required to maintain it over time is not included.

Table 4. Electricity consumption for PEC manufacturing, per m^2 PEC.

Exchange	Unit	PEC, BiVO4 photoanode	PEC, $TiFe_2O_5$ photoanode	Comments
$BiVO_4$ layer annealing	kWh	1.02		500°C, 2 hours according to TUM.
$TiFe_2O_5$ layer annealing	kWh		1.54	750°C, 8 hours, according to Avantama.
$CuFeO_2$ layer annealing	kWh	1.44	1.44	700°C, 30min, argon atmosphere, according to TUM.
Sputtering - FTO coating	kWh	6.7	6.7	24 MJ/m^2 according to Tsang (2016).
Sputtering- OPV	kWh	178	178	0.2174 kWh/nm of sputtered material, estimate by ICFO.
Roll-to-roll process	kWh	0.91	0.91	Includes solution preparation, layer coating and layer drying (zinc oxide and active layer). Drying accounts for 80% of the energy consumption. Values estimated by ICFO.
Thermal evaporation (Light management 2)	kWh	149	149	0.5233 kWh/nm of evaporated material of insulating nature (Molybdenum trioxide, lithium fluoride), estimate by ICFO.
Thermal evaporation (thin silver pellets)	kWh	2.3	2.3	0.2526 kWh/nm of evaporated material of conductive nature (silver), estimate by ICFO.
Gravure coating (thick silver connect ink)	kWh	0.26	0.26	Estimate by ICFO.
Encapsulation	kWh	0.0041	0.0041	Estimate by ICFO.
Total	kWh	339.3	339.8	

3.1.4 Manufacturing: waste and emissions

The quantification of waste and direct emissions by the PEC manufacturing process has been carried out based on a mass balance. The following aspects are included in the inventory:

- Emissions to air of solvents and argon (Table 5).
- Solid waste, mainly from the sputtering and thermal evaporation processes.

ICFO has provided an estimate of the amount of solid waste generated per m^2 PEC device, a total of 0.025 kg. The expected management of this waste is unclear. As a conservative assumption, and given that it is mainly constituted by inorganic materials, such as metal oxides, that cannot be used as fuel, it has been assumed that they can be sent to landfill. This is covered by means of an ecoinvent data set for inert waste disposal in Switzerland, which includes transport and landfilling according to an average Swiss scenario.

Table 5. Emissions to air from PEC manufacturing, per m^2 PEC.

Exchange	Unit	PEC, BiVO4 photoanode	PEC, $TiFe_2O_5$ photoanode	Comments
Emissions to air: solvents and argon				
Acetylacetone	kg	0.49		$BiVO_4$ synthesis solvent
Isopropanol	kg		0.00975	Pseudobrookite nanoparticles solvent
Ethanol	kg	0.083		FTO solution solvent
Water	kg	0.026		FTO solution solvent
2-methoxyethanol	kg	3.53E-06	3.53E-06	Zinc oxide solvent
Ethanolamine	kg	3.53E-08	3.53E-08	Zinc oxide additive
Chloroform	kg	5.08E-06	5.08E-06	Active layer solvent
Chloronaphthalene	kg	3.17E-08	3.17E-08	Active layer additive
Argon	kg	1.08	1.08	Argon used in sputtering
Emissions to air: atmospheric degradation of solvents				
Carbon dioxide, fossil	kg	1.08	0.02	Degradation of all solvents excluding ethanol
Carbon dioxide, biogenic	kg	0.16		Degradation of ethanol

The inventory in Table 5 includes not only the direct emissions of solvents, but also the CO_2 emissions as a result of the degradation of these solvents once in the atmosphere, mainly due to their interaction with hydroxyl radicals naturally present in the troposphere. The emission is calculated stoichiometrically from the carbon content of each solvent, based on their empirical formulae. It is assumed that all solvents are based on petrochemical derivatives, with the exception of ethanol, which is assumed to originate from fermentation of bio-based raw materials. For this reason, CO_2 emissions from ethanol are labelled as biogenic. Accounting for this CO_2 from atmospheric degradation can be argued to double-count emissions, since we have in the inventory parallel emissions of solvents and CO_2 from solvent degradation. This double-counting is required in order to capture in the study the contribution to greenhouse-gas (GHG) emissions from the use of these solvents, that would otherwise be omitted.

3.1.5 Manufacturing: overall inventory

Table 6 shows the overall inventory for PEC manufacturing as implemented in the life-cycle model. The reference flow is 1 m^2 PEC, which is estimated to weight 2.7 kg, of which 2.5 kg are constituted by the glass substrate used in the photoelectrode. The inventory includes an approximation for the following activities, not previously described:

- Manufacturing plant infrastructure: this is approximated with the ecoinvent data set for a photovoltaic panel factory. Consumption of this capital equipment is established in the ecoinvent database as 4E-06 factory units per m^2 photovoltaic panel produced. This same value is used in the inventory.
- Packaging materials: this is approximated with data extracted from the ecoinvent data set for manufacturing a liquid crystal display (LCD), where the packaging materials, namely cardboard and expanded polystyrene (EPS) are quantified at 0.132 kg and 0.162 kg, respectively, per kg product.

These figures are scaled up for 1 m^2 PEC weighting 2.7 kg. When this packaging is added, the weight of the packaged PEC is 3.5 kg/m^2.

- Transport of the finished PEC to the end user: this is approximated with the ecoinvent transport scenario for machinery, that includes transport services by road, sea, inland waters, air and rail. The inventory data for transporting 1 kg product are displayed in table Table 7.

All underlying data sets in Table 6 are either taken from the ecoinvent database, or derived specifically for this study. For certain chemical products, specific inventories were not derived, and the closest match in the ecoinvent database is used instead. This is the case for acetylacetone, 2-methoxyethanol and chloronaphthalene, covered by, respectively, acetone, a generic organic solvent, and O-chlorotoluene.

Table 6. Inventory data for PEC production, per m^2 PEC.

Exchange	**Unit**	**PEC ($BiVO_4$)**	**PEC ($TiFe_2O_5$)**	**Data set used and comments**
Outputs: Reference flow				
PEC, $BiVO_4$ {EU}	m^2 PEC	1		
PEC, $TiFe_2O_5$ {EU}	m^2 PEC		1	
Inputs: Products and services				
Glass substrate	kg	2.5	2.5	Solar glass, low-iron {GLO}| market for | Conseq, U
FTO solution	L	0.131	0.131	FTO solution {GLO} (LCI data in Table 13)
Bismuth nitrate	kg	0.025		Bismuth nitrate {GLO} (LCI data in Table 8)
Vanadyl acetylacetonate	kg	0.002		Vanadyl acetylacetonate {GLO} (LCI data in Table 10)
Acetylacetone	kg	0.49		Acetone, liquid {RER}| market for acetone, liquid | Conseq, U
Pseudobrookite nanoparticles dispersion	kg		0.01	Pseudobrookite nanoparticles, 2.5% w. dispersion {GLO} (LCI data in Table 17)
Iron oxides nanoparticles	kg	0.002	0.002	Iron oxides nanoparticles {GLO} (LCI data in Table 12)
Molecular catalyst	kg	0.003	0.003	Molecular catalyst {GLO} (LCI data in Table 16)
Copper nanoparticles	kg	0.00215	0.00215	Copper nanoparticles {GLO} (LCI data in Table 11)
PET substrate and encapsulation	kg	0.138	0.138	Polyethylene terephthalate, granulate, amorphous {GLO}| market for | Conseq, U
Light management 1 (SiO_2 target)	kg	0.00106	0.00106	Activated silica {GLO}| market for | Conseq, U
Light management 1 (TiO_2 target)	kg	0.0017	0.0017	Titanium dioxide {RER}| market for | Conseq, U
TRTC 1, 3 (zinc oxide target)	kg	0.000056	0.000056	Zinc oxide {GLO}| market for | Conseq, U
TRTC 2 (thin silver target), thin silver pellets, thick silver connect ink	kg	0.013	0.013	Silver {GLO}| market for | Conseq, U
Zinc acetate dihydrate	kg	0.00011	0.00011	Zinc acetate dihydrate {GLO} (LCI data in Table 20)
2-methoxyethanol (zinc oxide solvent)	kg	3.53E-06	3.53E-06	Solvent, organic {GLO}| market for | Conseq, U
Ethanolamine (zinc oxide additive)	kg	3.53E-08	3.53E-08	Diethanolamine {GLO}| market for | Conseq, U
Active layer (AL)	kg	0.000121	0.00021	PM6:Y6 active layer {GLO} (LCI data inTable 22)
Chloroform (AL solvent)	kg	5.08E-06	5.08E-06	Trichloromethane {RER}| market for trichloromethane | Conseq, U
Chloronaphthalene (AL additive)	kg	3.17E-08	3.17E-08	O-chlorotoluene {RER}| market for o-chlorotoluene | Conseq, U
Molybdenum trioxide, light management 2	kg	0.00049	0.00049	Molybdenum trioxide {GLO}| market for | Conseq, U
Light management 2 (Lithium fluoride)	kg	0.00048	0.00048	Lithium fluoride {GLO}| market for | Conseq, U

Adhesive epoxy	kg	0.029	0.029	Epoxy resin, liquid {RER}| market for epoxy resin, liquid | Conseq, U
Argon for sputtering	kg	1.08	1.08	Argon, liquid {RER}| market for argon, liquid | Conseq, U
Infrastructure	Unit	0.000004	0.000004	Photovoltaic panel factory {GLO}| market for | Conseq, U
Packaging, cardboard	kg	0.358	0.358	Folding boxboard/chipboard {GLO}| market for | Conseq, U
Packaging, expanded polystyrene	kg	0.438	0.438	Polystyrene, expandable {GLO}| market for | Conseq, U
Electricity	kWh	339.3	339.8	Electricity, medium voltage {Europe without Switzerland}| market group for | Conseq, U
Solid waste disposal	kg	0.025	0.025	Inert waste, for final disposal {CH}| market for inert waste, for final disposal | Conseq, U
Transport of finished product	kg	3.5	3.5	Transport, PEC {GLO} (LCI data in Table 7)
Outputs: Emissions to air				
Acetone	kg	0.49		$BiVO_4$ synthesis solvent
2-Propanol	kg		0.00975	Pseudobrookite nanoparticles solvent
Ethanol	kg	0.083		FTO solution solvent
Water	kg	0.026		FTO solution solvent
Ethanol, 2-methoxy-	kg	3.53E-06	3.53E-06	Zinc oxide solvent
Diethanolamine	kg	3.53E-08	3.53E-08	Zinc oxide additive
Chloroform	kg	5.08E-06	5.08E-06	Active layer solvent
Chloronaphthalene	kg	3.17E-08	3.17E-08	Active layer additive
Argon	kg	1.08	1.08	Argon used in sputtering
Carbon dioxide, fossil	kg	1.08	0.02	Atmospheric degradation of all solvents excluding ethanol
Carbon dioxide, biogenic	kg	0.16		Atmospheric degradation of ethanol

Table 7. Inventory data for PEC transport.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Transport, PEC {GLO}	kg	1	
Inputs: Products and services			
Train transport	tkm	0.018	Transport, freight train {GLO}| market group for | Conseq, U
Barge transport	tkm	0.001	Transport, freight, inland waterways, barge {GLO}| market group for transport, freight, inland waterways, barge | Conseq, U
Road transport	tkm	0.325	Transport, freight, lorry, unspecified {GLO}| market group for transport, freight, lorry, unspecified | Conseq, U
Maritime transport	tkm	0.737	Transport, freight, sea, container ship {GLO}| market for transport, freight, sea, container ship | Conseq, U
Air transport	tkm	0.018	Transport, freight, aircraft, unspecified {GLO}| market for transport, freight, aircraft, unspecified | Conseq, U

3.1.6 Bismuth nitrate

Bismuth nitrate, with the formula $Bi(NO_3)_3$, is a precursor for production of the $BiVO_4$ photoanode. The inventory for production of this chemical has taken as starting point the following chemical reaction (Yukhin et al. 2020), where bismuth reacts with nitric acid to form bismuth nitrate, water and nitrogen dioxide:

$$Bi + 6HNO_3 \rightarrow Bi(NO_3)_3 + 3H_2O + 3NO_2$$

Equation 2. Chemical reaction for production of bismuth nitrate.

From Equation 2 the stoichiometric amounts of raw materials and products has been obtained, while other inputs to the production process (energy, infrastructure) are approximated from the ecoinvent data set for production of potassium nitrate. A limitation to build this inventory is the fact that currently Bismuth production is not covered by the ecoinvent database. To overcome this gap, bismuth production is approximated by production of an alternative non-ferrous metal covered by the database, namely lead. Additionally, given the potentially high NO_x emissions, it has been assumed that these are partially abated by selective catalytic reduction (SCR), with an efficiency of 85%, as stated in the ecoinvent database for this technology. The remaining 15% is emitted to air. The final inventory data for Bismuth nitrate production are shown in Table 8. This includes transport of the final product, taking the same transport scenario as for chemicals in the ecoinvent database. These transport services, per kg product, are displayed in Table 9.

Table 8. Inventory data for Bismuth nitrate production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Bismuth nitrate {GLO}	kg	1	
Inputs: Products and services			
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| construction | Conseq, U
Bismuth	kg	0.53	Lead {GLO}| primary lead production from concentrate | Conseq, U
Nitric acid	kg	0.96	Nitric acid, without water, in 50% solution state {RER}| market for nitric acid, without water, in 50% solution state | Conseq, U
Thermal energy	MJ	4.56	Heat, district or industrial, natural gas {RER}| market group for | Conseq, U
NO_x abatement	kg	0.30	NOx retained, by selective catalytic reduction {GLO}| market for | Conseq, U
Wastewater treatment	L	0.14	Wastewater, unpolluted {RoW}| market for wastewater, unpolluted | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)
Outputs: emissions to air			
Nitrogen dioxide	kg	0.05	

Table 9. Inventory data for transport of chemical products to end user.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Transport, for chemicals {GLO}	kg	1	
Inputs: Products and services			
Train transport	tkm	0.309	Transport, freight train {GLO}| market group for | Conseq, U
Barge transport	tkm	0.025	Transport, freight, inland waterways, barge {GLO}| market group for transport, freight, inland waterways, barge | Conseq, U
Road transport	tkm	0.209	Transport, freight, lorry, unspecified {GLO}| market group for transport, freight, lorry, unspecified | Conseq, U
Maritime transport	tkm	0.599	Transport, freight, sea, container ship {GLO}| market for transport, freight, sea, container ship | Conseq, U

3.1.7 Vanadyl acetylacetonate

Vanadium(IV)-oxy acetylacetonate, with the formula $C_{10}H_{14}O_5V$, is a precursor for production of the $BiVO_4$ photoanode. The inventory for production of this chemical has taken as starting point the following chemical reaction (Rowe and Jones 1957), where vanadyl sulfate reacts with acetylacetone to produce Vanadyl acetylacetonate and sulfuric acid:

$VOSO_4 + 2\ C_5H_8O_2 \rightarrow C_{10}H_{14}O_5V + H_2SO_4$

Equation 3. Chemical reaction for production of vanadyl acetylacetonate.

From Equation 3 the stoichiometric amounts of raw materials and products has been obtained. Furthermore, the sulfuric acid by-product is assumed to be neutralized using sodium hydroxide:

$H_2SO_4 + 2\ NaOH \rightarrow Na_2SO_4 + 2H_2O$

Equation 4. Chemical reaction for sulfuric acid neutralization.

From Equation 4, the amount of sodium hydroxide is calculated stoichiometrically. Inputs of infrastructure, water and energy to the production process are approximated from the ecoinvent data set for production of acetyl chloride. For electricity, the global supply data set in ecoinvent is used. A limitation to build this inventory is the fact that neither vanadyl sulfate nor acetylacetone are covered by the ecoinvent database. To overcome this gap, vanadyl sulfate is approximated with the data set for magnesium sulfate, while production of acetylacetone is approximated with the data set for acetone. The final inventory data for are shown in Table 10. This includes transport of the final product.

Table 10. Inventory data for vanadyl acetylacetonate production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
vanadyl acetylacetonate {GLO}	kg	1	
Inputs: Natural resources			
Water, for cooling	L	24	
Inputs: Products and services			
Electricity	kWh	0.33	Electricity, medium voltage {GLO}| market group for | Conseq, U
Infrastructure	Unit	4.0E-10	Chemical factory, organics {RER}| construction | Conseq, U
Vanadyl sulfate	kg	0.95	Magnesium sulfate {GLO}| market for | Conseq, U
Acetylacetone	kg	0.75	Acetone, liquid {RoW}| market for acetone, liquid | Conseq, U
Thermal energy	MJ	2	Heat, from steam, in chemical industry {RoW}| market for heat, from steam, in chemical industry | Conseq, U
Sodium hydroxide	kg	0.30	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq, U
Transport of final product	kg	1	Transport, for chemicals (LCI data in Table 9)

3.1.8 Copper nanoparticles

Copper nanoparticles are delivered in the LICROX project by EPFL, however no primary data have been supplied to describe their production. Instead, the approach has been to look for literature data describing the production of such nanoparticles, and use these data as the best approximation available for the LICROX material. Inventory data on copper nanoparticle production have been obtained from Slotte and Zevenhoven (2017) for the arc process, where pure metal is evaporated through an electric discharge, condensed and recovered by filtration. The metal is kept under an inert atmosphere at atmospheric or a slight under-pressure. A flow diagram for this process is shown in Figure 5. It must be highlighted that these data do not reflect industrial-scale production, but rather an experimental setup.

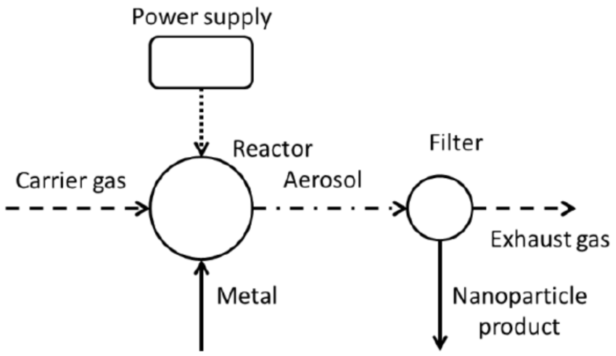

Figure 5. arc/spark setup for nanoparticle production (Slotte and Zevenhoven 2017).

Slotte and Zevenhoven (2017) report the use of energy and the mass balance for the production process, including the production of waste copper that is assumed by the authors to be recycled. We added inputs of infrastructure assuming the same figures as in organic chemicals in the ecoinvent database, as well as the transport of the finished product. For electricity supply, the global supply mix in the ecoinvent database is used. The inventory data are shown in Table 11, per gram of copper nanoparticles.

Table 11. Inventory data for copper nanoparticles production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Copper nanoparticles {GLO}	g	1	
Inputs: Products and services			
Electricity	kWh	0.139	Electricity, medium voltage {GLO}| market group for | Conseq, U
Infrastructure	Unit	4.0E-13	Chemical factory, organics {RER}| construction | Conseq, U
Copper	g	5.26	Copper {GLO}| market for | Conseq, U
Nitrogen	g	0.52	Nitrogen, liquid {RER}| market for | Conseq, U
Copper waste, to recycling	g	4.22	Copper scrap, sorted, pressed {RER}| treatment of copper scrap by electrolytic refining | Conseq, U
Transport of final product	g	1	Transport, for chemicals {GLO} (LCI data in Table 9)

3.1.9 Iron oxides nanoparticles

Iron oxides nanoparticles are used as a precursor of the $CuFeO_2$ photocathode and they are delivered into the LICROX project by EPFL. The approach to include the production of this material in the study is similar to that followed for the production of copper nanoparticles, that is, to look for literature data on their production. This is provided by Patiño-Ruiz et al. (2021), where an inventory is reported for the production of iron oxide through the co-precipitation method. However, the data have been discarded as they seem to reflect a lab-scale process without any effort in up-scaling. This leads to what in our opinion are unrealistic figures, such as an electricity consumption of 8 GWh per kg nanoparticles. Instead, we have opted for using the data reported by Marimón-Bolívar and González (2018) for production of Fe_3O_4 nanoparticles using the same co-precipitation method. In this case, though, energy consumption is estimated theoretically, leading to more reasonable figures. Consumption of reagents still reflects lab-scale experiments, though.

The production process described by Marimón-Bolívar and González (2018) has inputs of iron (II) chloride, iron (III) chloride, a 30% solution of ammonium hydroxide and water. Water is included in the model as tap water, while the ammonium hydroxide solution is included as a 30% solution of ammonia and ultrapure water. The energy inputs are electricity and thermal energy from natural gas. A mass balance is used to determine the amount of wastewater generated, which is included in the model with a generic data set for urban wastewater treatment in ecoinvent. We also added inputs of infrastructure assuming the same figures as in organic chemicals in the ecoinvent database, as well as the transport of the finished product. The inventory data for producing 1 g iron oxides nanoparticles are shown in Table 12.

Table 12. Inventory data for iron oxides nanoparticles production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Iron oxides nanoparticles {GLO}	g	1	
Inputs: Products and services			
Iron (II) chloride	g	0.46	Iron(II) chloride {GLO}| market for | Conseq, U
Iron (III) chloride	g	0.9	Iron(III) chloride, without water, in a 12% iron solution state {GLO}| market for | Conseq, U
Ammonia	kg	0.027	Ammonia, liquid {RoW}| market for | Conseq, U
Water for ammonia dilution	L	0.063	Water, ultrapure {RoW}| market for water, ultrapure | Conseq, U
Tap water	L	207	Tap water {Europe without Switzerland}| market for | Conseq, U
Thermal energy	MJ	0.047	Heat, district or industrial, natural gas {RoW}| market group for | Conseq, U
Electricity	kWh	0.0128	Electricity, medium voltage {GLO}| market group for | Conseq, U
Infrastructure	Unit	4.0E-13	Chemical factory, organics {RER}| construction | Conseq, U
Wastewater treatment	L	0.297	Wastewater, average {Europe without Switzerland}| market for wastewater, average | Conseq, U
Transport of final product	g	1	Transport, for chemicals {GLO} (LCI data in Table 9)

3.1.10 Fluorine-doped tin oxide

According to TUM, the glass substrate in the photoelectrode needs to be coated with a 500 nm layer of fluorine doped tin oxide (FTO). Production of this coating is described by Tsang (2016) as a solution using the precursors tin tetrachloride and ammonium fluoride mixed with 80:20 ethanol:water. The inventory for this solution is shown in table Table 13, per L solution, while Table 14 and Table 15 show the corresponding inventories for production of the precursors ammonium fluoride and tin tetrachloride, respectively, as these materials are not currently covered by the ecoinvent database. These inventories are also based on data reported by Tsang (2016). All products include an input of infrastructure which is used in the ecoinvent database for all chemical production processes, as well as the transport of the final product.

Table 13. Inventory data for FTO solution production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
FTO solution {GLO}	L	1	
Inputs: Products and services			
Ammonium fluoride	kg	0.014	Ammonium fluoride {GLO} (LCI data in Table 14)
Ethanol	kg	0.63	Ethanol, without water, in 99.7% solution state, from fermentation {GLO}| market for | Conseq, U
Thermal energy	MJ	298	Heat, district or industrial, other than natural gas {RoW}| heat production, heavy fuel oil, at industrial furnace 1MW | Conseq, U
Tin tetrachloride	kg	0.078	Tin tetrachloride {GLO} (LCI data in Table 15)
Deionised water	L	0.2	Water, deionised {RoW}| market for water, deionised | Conseq, U
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| market for | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

Table 14. Inventory data for ammonium fluoride production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Ammonium fluoride {GLO}	kg	1	
Inputs: Products and services			
Ammonia	kg	0.46	Ammonia, liquid {RoW}| market for | Conseq, U
Thermal energy	MJ	0.57	Heat, district or industrial, other than natural gas {RoW}| heat production, heavy fuel oil, at industrial furnace 1MW | Conseq, U
Hydrogen fluoride	Kg	0.54	Hydrogen fluoride {RoW}| market for hydrogen fluoride | Conseq, U
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| market for | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

Table 15. Inventory data for Tin tetrachloride production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Tin tetrachloride {GLO}	kg	1	
Inputs: Products and services			
Chlorine	kg	0.54	Chlorine, liquid {RoW}| market for chlorine, liquid | Conseq, U
Thermal energy	MJ	0.13	Heat, district or industrial, other than natural gas {RoW}| heat production, heavy fuel oil, at industrial furnace 1MW | Conseq, U
Tin	Kg	0.46	Tin {GLO}| market for | Conseq, U
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| market for | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

3.1.11 Molecular catalysts

Molecular iron complexes are used in the PEC photocathode as catalysts to perform the reduction of CO_2 into ethylene. These catalysts are delivered to the LICROX project by ICIQ, which plans to produce two types of molecules based on iron. However, details have only been provided for one of them, which is used in the study to represent both. The targeted molecule is iron(tetraphenylporphyrinato) chloride, or Fe(TPP)Cl (Figure 6).

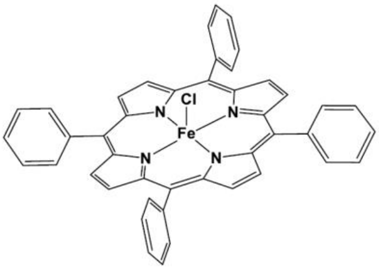

Figure 6. Chemical structure of iron(tetraphenylporphyrinato) chloride.

This chemical compound is currently not covered by the ecoinvent database, and for this reason an attempt has been made to estimate an inventory for its production. A mass balance has been developed considering the synthesis in two steps:

- Production of the precursor tetraphenylporphyrin from pyrrole and benzaldehyde, following the Rothemund reaction.
- Production of Fe(TPP)Cl by the reaction of tetraphenylporphyrin and ferrous chloride.

These two chemical reactions are shown in Equation 5 and Equation 6:

$$8C_4H_5N + 8C_7H_6O + 3O_2 \rightarrow 2C_{44}H_{30}N_4 + 14H_2O$$

Equation 5. Chemical reaction for production of tetraphenylporphyrin.

$$C_{44}H_{30}N_4 + FeCl_2 + \tfrac{1}{4}\,O_2 \rightarrow C_{44}H_{28}ClFeN_4 + HCl + \tfrac{1}{2}\,H_2O$$

Equation 6. Chemical reaction for production of iron(tetraphenylporphyrinato) chloride.

The mass balance is built as the sum of these two reactions, assuming in both cases a yield of 100%. Pyrrole production, which is currently not covered by the ecoinvent database, is approximated by production of pyridine, a similar heterocyclic organic compound containing nitrogen, for which data are available in the database. The hydrogen chloride by-product in Equation 6 is assumed to require neutralization by sodium hydroxide. The amount of sodium hydroxide is calculated stoichiometrically from Equation 7:

$$HCl + NaOH \rightarrow NaCl + H_2O$$

Equation 7. Chemical reaction for hydrochloric acid neutralization.

Besides the final Fe(TPP)Cl product, the sum of water and sodium chloride from neutralization is modelled as urban wastewater for treatment. No other material inputs are included, besides infrastructure. Regarding energy consumption, this is coarsely estimated for the net reaction with the same amount of electricity and steam required for production of unspecified pesticides according to the ecoinvent database. This can be thought of representing the energy expenditures for manufacturing a complex organic chemical, however with substantial uncertainty involved. The overall inventory data, including transport of the finished product, are shown in Table 16.

Table 16. Inventory data for molecular catalyst production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Fe(TPP)Cl {GLO}	kg	1	
Inputs: Products and services			
Pyrrole	kg	0.381	Pyridine {GLO}| market for | Conseq, U
Benzaldehyde	kg	0.603	Benzaldehyde {RoW}| market for benzaldehyde | Conseq, U
Oxygen	kg	0.080	Oxygen, liquid {RoW}| market for | Conseq, U
Ferrous chloride	kg	0.181	Iron(II) chloride {GLO}| market for | Conseq, U
Sodium hydroxide	kg	0.057	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq, U
Electricity	kWh	1.93	Electricity, medium voltage {GLO}| market group for | Conseq, U
Thermal energy	MJ	24.16	Heat, from steam, in chemical industry {RoW}| market for heat, from steam, in chemical industry | Conseq, U
Wastewater for treatment	L	0.301	Wastewater, average {RoW}| market for wastewater, average | Conseq, U
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| market for | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

3.1.12 Pseudobrookite nanoparticles

Pseudobrookite (Fe_2TiO_5) nanoparticles are proposed in the LICROX project as an alternative photoanode material to $BiVO_4$. These nanoparticles are delivered to the project by Avantama, which has provided primary data for small-scale production of these nanoparticles as a dispersion in isopropanol, containing 2.5% nanoparticles in weight. The primary data supplied by Avantama included the use of chemical precursors, solvents, energy, process emissions and waste generation. The inventory data are shown in Table 17, where the reference flow is the weight of dispersion (40 g) containing 1 g nanoparticles.

Table 17. Inventory data for pseudobrookite nanoparticles production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Pseudobrookite nanoparticles, 2.5% w. dispersion {GLO}	g	40	
Inputs: Products and services			
Oxygen	kg	0.060	Oxygen, liquid {RoW}| market for | Conseq, U
Thermal energy	MJ	0.166	Heat, district or industrial, natural gas {GLO}| market group for | Conseq, U
Tap water	kg	0.05	Tap water {RoW}| market for | Conseq, U
Electricity	kWh	0.435	Electricity, medium voltage {GLO}| market group for | Conseq, U
2-Ethylhexanoic acid	g	7.5	Benzoic acid {RoW}| market for benzoic acid | Conseq, U
Xylenes	g	5	Xylene {RoW}| market for xylene | Conseq, U
Ferrous acetate	g	1	Ferrous acetate {GLO} (LCI data in Table 19)
Titanium isopropoxide	g	1.5	Titanium isopropoxide {GLO} (LCI data in Table 18)
Isopropanol	kg	1.57	Isopropanol {RoW}| market for isopropanol | Conseq, U
Wastewater, for treatment	L	0.05	Wastewater, average {RoW}| market for wastewater, average | Conseq, U
Chemical waste, for disposal	kg	1.5	Hazardous waste, for incineration {RoW}| market for hazardous waste, for incineration | Conseq, U
Infrastructure	Unit	1.6E-11	Chemical factory, organics {GLO}| construction | Conseq, U
Transport of final product	kg	0.040	Transport, for chemicals {GLO} (LCI data in Table 9)

Two of the chemical precursors involved in the production of these nanoparticles, namely titanium isopropoxide and ferrous acetate, are not currently covered by the ecoinvent database. The inventories for their production have been approximated as described below.

Titanium isopropoxide, with the formula Ti {OCH $(CH_3)_2$} $_4$, is produced by treating titanium tetrachloride with isopropanol, with hydrogen chloride being formed as a by-product (Bradley et al. 2001):

$$TiCl_4 + 4\ (CH_3)_2CHOH \rightarrow Ti\{OCH(CH_3)_2\}_4 + 4\ HCl$$

Equation 8. Chemical reaction for production of titanium isopropoxide.

The inventory for production of this chemical has taken as starting point the stoichiometry in Equation 8, assuming a yield of 100%. Furthermore, the hydrochloric acid by-product is assumed to be neutralized using sodium hydroxide, as previously shown in Equation 7. Inputs of water, energy (electricity and heat) as well as infrastructure are approximated with the same data as in the data set for production of isopropyl acetate in the ecoinvent database. The final inventory data for titanium isopropoxide production are shown in Table 18, including transport of the final product.

Table 18. Inventory data for titanium isopropoxide production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Titanium isopropoxide {GLO}	kg	1	
Inputs: Natural resources			
Cooling water	m^3	0.024	
Inputs: Products and services			
Titanium tetrachloride	kg	0.669	Titanium tetrachloride {GLO}| market for | Conseq, U
Isopropanol	kg	0.845	Isopropanol {RoW}| market for isopropanol | Conseq, U
Sodium hydroxide	kg	0.563	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq, U
Electricity	kWh	0.079	Electricity, medium voltage {GLO}| market group for | Conseq, U
Thermal energy	MJ	6.72	Heat, district or industrial, natural gas {GLO}| market group for | Conseq, U
Thermal energy	MJ	3.75	Heat, district or industrial, other than natural gas {GLO}| market group for | Conseq, U
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| construction | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

Ferrous acetate, with the formula $Fe(CH_3CO_2)_2$, is produced by electrolysis from the reaction of iron powder with acetic acid, forming ferrous acetate and hydrogen gas (Weber et al. 2011):

$$Fe + 2\ CH_3CO_2H \rightarrow Fe(CH_3CO_2)_2 + H_2$$

Equation 9. Chemical reaction for production of ferrous acetate.

The inventory for production of this chemical has taken as starting point the stoichiometry in Equation 9, assuming a yield of 100%. Inputs of water, energy (electricity and heat) as well as infrastructure and solid waste are approximated with the same data as in the data set for production of iron (III) sulfate in the ecoinvent database. The final inventory data for ferrous acetate production are shown in Table 19, including transport of the final product.

Table 19. Inventory data for ferrous acetate production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Ferrous acetate {GLO}	kg	1	
Inputs: Products and services			
Iron powder	kg	0.322	Magnetite {GLO}| market for | Conseq, U
Acetic acid	kg	0.690	Acetic acid, without water, in 98% solution state {GLO}| market for | Conseq, U
Tap water	kg	0.134	Tap water {GLO}| market group for | Conseq, U
Deionised water	kg	0.086	Water, deionised {RoW}| market for water, deionised | Conseq, U
Electricity	kWh	0.031	Electricity, medium voltage {GLO}| market group for | Conseq, U
Thermal energy	MJ	0.026	Heat, district or industrial, natural gas {GLO}| market group for | Conseq, U
Solid waste for disposal	kg	0.011	Sludge, pig iron production {RoW}| treatment of, residual material landfill | Conseq, U
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| construction | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)
Outputs: Emissions to air			
Hydrogen	kg	0.011	

3.1.13 Zinc acetate dihydrate

Zinc acetate dihydrate, with the formula $Zn(CH_3COO)_2$, is a component of the OPV. The inventory for production of this chemical has taken as starting point the following chemical reaction (Sciencemadness 2019), where acetic acid reacts with zinc oxide to form zinc acetate and water:

$$2\ CH_3COOH + ZnO + H_2O \rightarrow Zn(CH_3COO)_2 \cdot 2H_2O$$

Equation 10. Chemical reaction for production of zinc acetate.

From Equation 10 the stoichiometric amounts of raw materials and products has been obtained, while other inputs to the production process (energy, auxiliary materials, infrastructure) are approximated from the ecoinvent data set for production of iron (III) sulfate. The final inventory data for zinc acetate production, inculding transport of the final product, are shown in Table 20.

Table 20. Inventory data for zinc acetate production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Zinc acetate dihydrate {GLO}	kg	1	
Inputs: Products and services			
Zinc oxide	kg	0.37	Zinc oxide {GLO}| market for | Conseq, U
Acetic acid	kg	0.55	Acetic acid, without water, in 98% solution state {GLO}| market for | Conseq, U
Tap water	kg	0.134	Tap water {GLO}| market group for | Conseq, U
Deionised water	kg	0.086	Water, deionised {RoW}| market for water, deionised | Conseq, U
Electricity	kWh	0.031	Electricity, medium voltage {GLO}| market group for | Conseq, U
Thermal energy	MJ	0.026	Heat, district or industrial, natural gas {GLO}| market group for | Conseq, U
Solid waste for disposal	kg	0.011	Sludge, pig iron production {RoW}| treatment of, residual material landfill | Conseq, U
Infrastructure	kg	4E-10	Chemical factory, organics {GLO}| market for | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

3.1.14 Active layer polymers

The OPV uses a PM6:Y6 material combination in its active layer, as opposed to inorganic materials like silicon in conventional photovoltaics. The polymer PM6, also named PBDB-TF or PBDB-T2F is used as electron donor, while Y6, also named BTP 4-F, acts as electron acceptor.

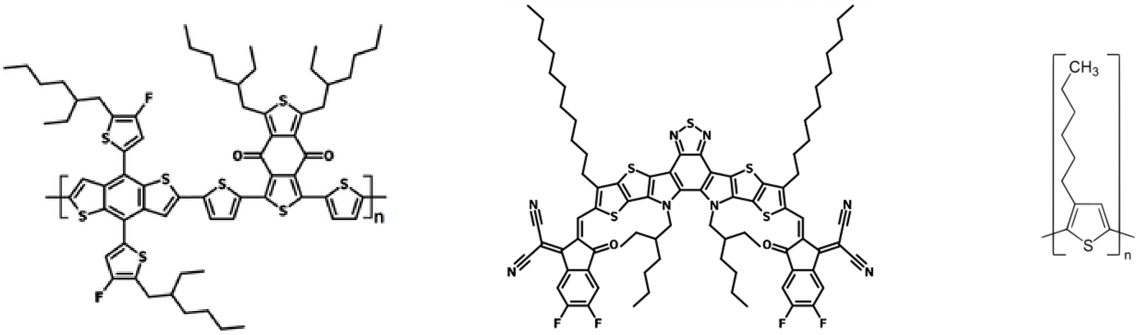

Figure 7. Chemical structure of PM6 (left), Y6 (centre) and P3HT (right).

We have not been able to find inventory data for neither of these polymers. Their production has been approximated with data for the production of poly(3-hexylthiophene-2,5-diyl) or P3HT, another polymer commonly used in the active layer of organic photovoltaics, which is also based on thiophene, and for which detailed inventory data are provided by Tsang (2016). The author provides the inventory in two steps: production of thiophene and production of P3HT. The inventory for production of thiophene from butane and sulfur was developed by Tsang (2016) with data from a US patent and from the Ullmann's Encyclopedia of Industrial Chemistry, while the inventory for P3HT as a reaction of thiophene, bromine and hexane was developed with data from García-Valverde et al. (2010). The data for these two production steps are shown in Table 21 and Table 22, respectively.

Table 21. Inventory data for thiophene production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Thiophene {GLO}	kg	1	
Inputs: Products and services			
Aluminium oxide	kg	0.4	Aluminium oxide, non-metallurgical {RoW}| market for aluminium oxide, non-metallurgical | Conseq, U
Butane	kg	0.69	Butane {GLO}| market for | Conseq, U
Chromium oxide	kg	0.8	Chromium oxide, flakes {GLO}| market for | Conseq, U
Thermal energy	MJ	1.81	Heat, district or industrial, other than natural gas {RoW}| heat production, heavy fuel oil, at industrial furnace 1MW | Conseq, U
Hydrogen sulfide	kg	1.22	Hydrogen sulfide {RoW}| market for hydrogen sulfide | Conseq, U
Sulfur	kg	1.52	Sulfur {GLO}| market for | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

Table 22. Inventory data for PM6:Y6 active layer production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
PM6:Y6 active layer {GLO}	kg	1	
Inputs: Products and services			
Thiophene	kg	7.81	Thiophene {GLO} (LCI data in Table 21)
Bromine	kg	8.97	Bromine {GLO}| market for | Conseq, U
Electricity	kWh	36.4	Electricity, medium voltage {GLO}| market group for | Conseq, U
Thermal energy	GJ	1.15	Heat, district or industrial, other than natural gas {RoW}| heat production, heavy fuel oil, at industrial furnace 1MW | Conseq, U
Hexane	kg	2.58	Hexane {GLO}| market for | Conseq, U
Water	m^3	11.14	Water, ultrapure {RER}| market for water, ultrapure | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

3.2 LICROX plant infrastructure

Data on the design of an ethylene production plant based on the LICROX concept were not available by the consortium. An attempt has been made to include this aspect in the study, by quantifying infrastructure for two separate parts of the plant:

- PEC infrastructure, understood as the materials and equipment, other than the PEC themselves, to support plant operation.
- DSP infrastructure, characterized according to the consortium as a pressure swing adsorption unit.

A description of the inventory data, calculations and assumptions for these two parts of the plant is given in sections 3.2.1 and 3.2.2. Both infrastructure data sets include the iLUC effects from land occupation. This particular aspect of the inventory is described in section 3.2.3.

3.2.1 Photoelectrochemical cell plant infrastructure

Infrastructure for a solar-based installation of PEC devices is approximated based on data for the plant described by Muñoz (2006). This is a full-scale demonstration plant in Southern Spain (Almería region), applying solar photocatalysis by the photo-Fenton reaction, to treat industrial wastewaters, using a solar field of compound parabolic collectors (CPC). Table 23 shows the underlying data by Muñoz (2006) for this photocatalysis plant, where all materials were reported per 1 m^2 of installed CPC, which is equivalent in the present study to 1 m^2 PEC. In order to annualize the consumption of materials, a service life has been assumed. This is 30 years for structural materials, pipes, tanks, etc., and 10 years for machinery and equipment.

Table 23. Land occupation and list of materials considered in the LICROX plant infrastructure.

Component	**Unit**	**Amount**	**Service life**	**Comments**
Stainless steel	kg/m^2 PEC	7.81	30	Structural elements such as supports, plates, screws.
Aluminium	kg/m^2 PEC	6.43	30	Structural elements, namely CPC frames. Aluminium for CPC mirrors are excluded as this is not part of the LICROX concept.
Galvanized steel	kg/m^2 PEC	0.17	30	Screws and minor structural elements.
Polypropylene	kg/m^2 PEC	2.225	30	Pipes, tanks and valves in polypropylene.
Glass fibre reinforced plastic	kg/m^2 PEC	1.24	30	For tanks.
Concrete	m^3/m^2 PEC	0.32	30	For paved floor.
Reinforcing steel	kg/m^2 PEC	31	30	Concrete reinforcement.
Concrete blocks	kg/m^2 PEC	46	30	Paved floor perimeter.
Pumps	kg/m^2 PEC	0.293	10	Total weight of pumps for water circulation and chemical dosing.
Control unit	kg/m^2 PEC	0.33	10	Control box.

The data in Table 23 is the basis for the LICROX PEC infrastructure inventory shown in Table 24. The inventory for plastics includes the production of the polymers as well as their processing, approximated by the extrusion process for plastic pipes in the ecoinvent database. In the particular case of pumps, the weight in Table 23 has been transformed into units of pumps, as the reference flow for the model pump in the ecoinvent database is 1 unit of pump, weighting 2.43 kg. In Table 24 the reference flow is using 1 m^2 PEC during 1 year, or 1 m^2 PEC-year.

Table 24. Inventory data for LICROX PEC infrastructure.

Exchange	**Unit**	**Amount**	**Data set used and comments**
Outputs: Reference flow			
LICROX PEC infrastructure {EU}	m^2 PEC-year	1	Using 1 m^2 PEC during 1 year
Inputs: Natural resources			
Land occupation, industrial area	m^{2}year	3.25	
Inputs: Products and services			
iLUC, arable land	kg NPP$_0$ as C	1.92	Arable land, as NPP$_0$ {GLO} (LCI data in Table 27)
Stainless steel	kg	0.260	Steel, chromium steel 18/8, hot rolled {GLO}| market for | Conseq, U
Aluminium	kg	0.214	Aluminium, wrought alloy {GLO}| market for | Conseq, U
Galvanized steel	kg	0.006	Steel, low-alloyed {GLO}| market for | Conseq, U
Polypropylene	kg	0.074	Polypropylene, granulate {GLO}| market for | Conseq, U
Glass fibre reinforced plastic	kg	0.041	Glass fibre reinforced plastic, polyester resin, hand lay-up {GLO}| market for | Conseq, U
Plastics processing	kg	0.116	Extrusion, plastic pipes {GLO}| market for | Conseq, U
Concrete	m^3	0.011	Concrete, normal {CH}| market for | Conseq, U
Reinforcing steel	kg	1.033	Reinforcing steel {GLO}| market for | Conseq, U
Concrete block	kg	46	Concrete block {DE}| market for concrete block | Conseq, U
Pumps	Unit	0.0121	Pump, 40W {GLO}| market for | Conseq, U
Control unit	kg	0.033	Electronics, for control units {GLO}| market for | Conseq, U

3.2.2 Downstream processing plant infrastructure

According to the LICROX consortium, the DSP infrastructure can be best approximated by an industrial PSA unit. Inventory data for such a plant has been reported by Kohlheb et al. (2021) for a PSA unit designed to purify biogas. The authors provided a detailed bill of materials, their useful life in years, and the total volume of gas processed during the useful life of the plant (233.6 million Nm^3 biogas in 20 years). Thus, the infrastructure requirements can be derived per Nm^3 processed gas, which is used as reference flow in Table 25, where the inventory is displayed.

Kholheb et al. did not report on the land occupation requirements for such a plant. In order to capture this aspect in the inventory, this has been quantified with expert judgement from Hysytech, suggesting that the DSP unit would probably not use more than 5% of the total LICROX plant requirements, with the remaining 95% corresponding to the PEC infrastructure. The estimated land occupation, expressed per Nm^3 gas input to the DSP unit is 0.75 m^2-year.

Table 25. Inventory data for LICROX DSP infrastructure.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
LICROX DSP infrastructure {EU}	Nm^3 gas input	1	1 Nm^3 gas input to the PSA unit
Inputs: Natural resources			
Land occupation, industrial area	m^{2}year	0.75	
Inputs: Products and services			
iLUC, arable land	kg NPP$_0$ as C	0.44	Arable land, as NPP$_0$ {GLO} (LCI data in Table 27)
Excavation	m3	2.32E-10	Excavation, hydraulic digger {GLO}| market for | Conseq, U
Gravel	kg	0.00078	Gravel, crushed {RoW}| market for gravel, crushed | Conseq, U
Concrete	m3	3.52E-07	Concrete, normal {RoW}| market for | Conseq, U
Steel	kg	0.00020	Steel, low-alloyed {GLO}| market for | Conseq, U
Messing	kg	6.42E-09	Brass {RoW}| market for brass | Conseq, U
PP	kg	4.14E-05	Propylene, petrochemical {EU}
PP pipe extrusion	kg	4.14E-05	Extrusion, plastic pipes {RER}| extrusion, plastic pipes | Conseq, U
Pump	Units	9.31E-07	Water pump, 22kW {GLO}| market for water pump, 22kW | Conseq, U
Chiller	Units	1.03E-08	Absorption chiller, 100kW {GLO}| market for | Conseq, U
Compressor	Units	1.40E-08	Air compressor, screw-type compressor, 300kW {GLO}| market for | Conseq, U
Aluminium	kg	4.71E-09	Aluminium, wrought alloy {GLO}| market for | Conseq, U
Activated carbon	kg	0.00029	Activated carbon, granular {GLO}| market for activated carbon, granular | Conseq, U
Aluminium oxide	kg	1.19E-07	Aluminium oxide, non-metallurgical {IAI Area, EU27 & EFTA}| market for aluminium oxide, non-metallurgical | Conseq, U
Expansion vessel	Units	9.59E-08	Expansion vessel, 80l {GLO}| market for | Conseq, U
Water	kg	2.40E-05	Tap water {RER}| market group for | Conseq, U
Glycol	kg	1.15E-05	Ethylene glycol {GLO}| market for | Conseq, U
Lubricating oil	kg	7.71E-06	Lubricating oil {RER}| market for lubricating oil | Conseq, U

3.2.3 Indirect land use change

iLUC is linked to the demand for land by the LICROX plant. As described in section 2.10.2, the default assumption in this study is that industrial activities expand on land that was previously used for agriculture. The iLUC flow in the inventory is quantified as a demand for productive capacity from arable land with an average production capacity of 591 g carbon/m^2-year. This value has been calculated for this study as a weighted average for the EU27, considering the area of cropland and its productive capacity, in g carbon/m^2-year, for each member state. The calculation is shown in Table 26. In this table, the data for each member state was obtained by a detailed overlay analysis in a geographic information system (GIS), using a 10 x 10 km grid of potential NPP$_0$ (Haberl et al. 2007), a 0.05 x 0.05 km grid of land cover data (Friedl et al. 2010) and national borders.

Table 26. Calculating the potential primary production (NPP$_0$) of cropland in the EU27.

Component	Cropland area (m^2)	NPP$_0$ (g carbon/m^2-year)	NPP$_0$ (g carbon/year)
Austria	1.30E+10	650	8.46E+12
Belgium	9.47E+09	632	5.98E+12
Bulgaria	6.48E+10	540	3.50E+13
Cyprus	3.52E+09	410	1.44E+12
Czech Republic	2.47E+10	628	1.55E+13
Germany	1.19E+11	615	7.32E+13
Denmark	2.59E+10	615	1.59E+13
Estonia	1.31E+09	578	7.59E+11
Spain	1.50E+11	532	7.97E+13
Finland	1.66E+09	529	8.78E+11
France	2.41E+11	659	1.59E+14
Greece	4.71E+10	449	2.12E+13
Hungary	6.54E+10	609	3.98E+13
Ireland	3.28E+09	619	2.03E+12
Italy	1.29E+11	556	7.18E+13
Lithuania	2.32E+10	615	1.43E+13
Luxembourg	4.01E+08	637	2.56E+11
Latvia	7.02E+09	604	4.24E+12
Malta	9.94E+07	410[a]	4.08E+10
Netherlands	1.00E+10	594	5.97E+12
Poland	1.41E+11	638	9.01E+13
Portugal	2.25E+10	557	1.25E+13
Romania	1.21E+11	518	6.29E+13
Sweden	1.01E+10	613	6.18E+12
Slovenia	2.52E+09	687	1.73E+12
Slovakia	1.76E+10	641	1.13E+13
Croatia	1.72E+10	659	1.13E+13
EU27	**1.27E+12**	**591**	**7.52E+14**

[a] No data available for Malta. Approximated with the same value as Cyprus.

With an average productivity of 0.591 kg C/m^2-year, the occupation of 1 such m^2 for a year entails a demand of 1/0.591 = 1.69 kg NPP$_0$ as carbon. In the model by Schmidt et al. (2015) a demand for 1 kg NPP$_0$ from arable land is fulfilled partially by land transformation (deforestation) and partially by intensification of arable land already in use. This is captured in Table 27. On the one hand, land transformation leads to a conversion of previously forested land into cropland, with derived carbon dioxide emissions from carbon stock changes. On the other hand, intensification of arable land already in use is modelled as an increase in the use of nitrogen fertilisers, and their derived emissions after application to soil. Supply of nitrogen is modelled as supply of urea, as this is the nitrogen fertiliser with the highest production growth trend in the period 2007-2016, based on data from the International Fertiliser Association (IFASTAT 2019).

Table 27. Inventory data for indirect land use change in arable land.

Activity	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Arable land, as NPP_0 {GLO}	Kg NPP_0 as C	1	
Inputs: Natural resources			
Occupation, accelerated denaturalisation, secondary forest to arable	m^2-yr	0.539	From land transformation
Inputs: Products and services			
N fertilizer	kg	0.0096	Urea, as N {GLO}| market for | Conseq, U
Outputs: Emissions to air			
Carbon dioxide	kg	0.18	From land transformation
Ammonia	kg	1.15E-03	From intensification
Dinitrogen monoxide	kg	2.21E-04	From intensification
Nitrogen oxides	kg	5.56E-05	From intensification
Outputs: Emissions to water			
Nitrate	kg	0.0142	From intensification

3.3 LICROX plant operation

Operation of the LICROX plant includes the following aspects:

- Supply of industrial CO_2.
- Supply of ultrapure water.
- Supply of potassium bicarbonate.
- Supply of electricity.
- Supply of tap water.
- Downstream processing of the obtained gases.
- Management of spent electrolyte as wastewater.

Based on the primary data supplied by the LICROX consortium on the above aspects, a mass and energy balance has been established, as shown in Figure 8. The expected ethylene yield by the PEC device is 0.015 kg/m^2 PEC-day. With this figure, and taking into account the chemical reaction involved (Equation 1), stoichiometric amounts of CO_2 and water inputs, as well as O_2 output, can be calculated. The net CO_2 input to the plant as well as the amount recirculated from the DSP unit is calculated assuming that the CO_2 utilization efficiency at each pass through the PEC is 8%, but 80% when recirculation of this gas is considered. The remaining 20% is lost to the atmosphere from the DSP unit, according to the consortium. Inputs of water include the stoichiometric amount needed for the chemical reaction, as well as the volume in the electrolyte, which is continuously recirculated from the DSP unit back to the PEC. The volume of water and potassium bicarbonate needed per kg ethylene produced is calculated based on the total amounts needed and the frequency of replacement, which assumed to be on a weekly basis. This electrolyte is discharged and treated as wastewater. Regarding energy, the net flow of solar energy is quantified as the amount ultimately embedded in the ethylene product (high calorific value), while the total grid electricity demand by the plant is estimated as 5.4 kWh.

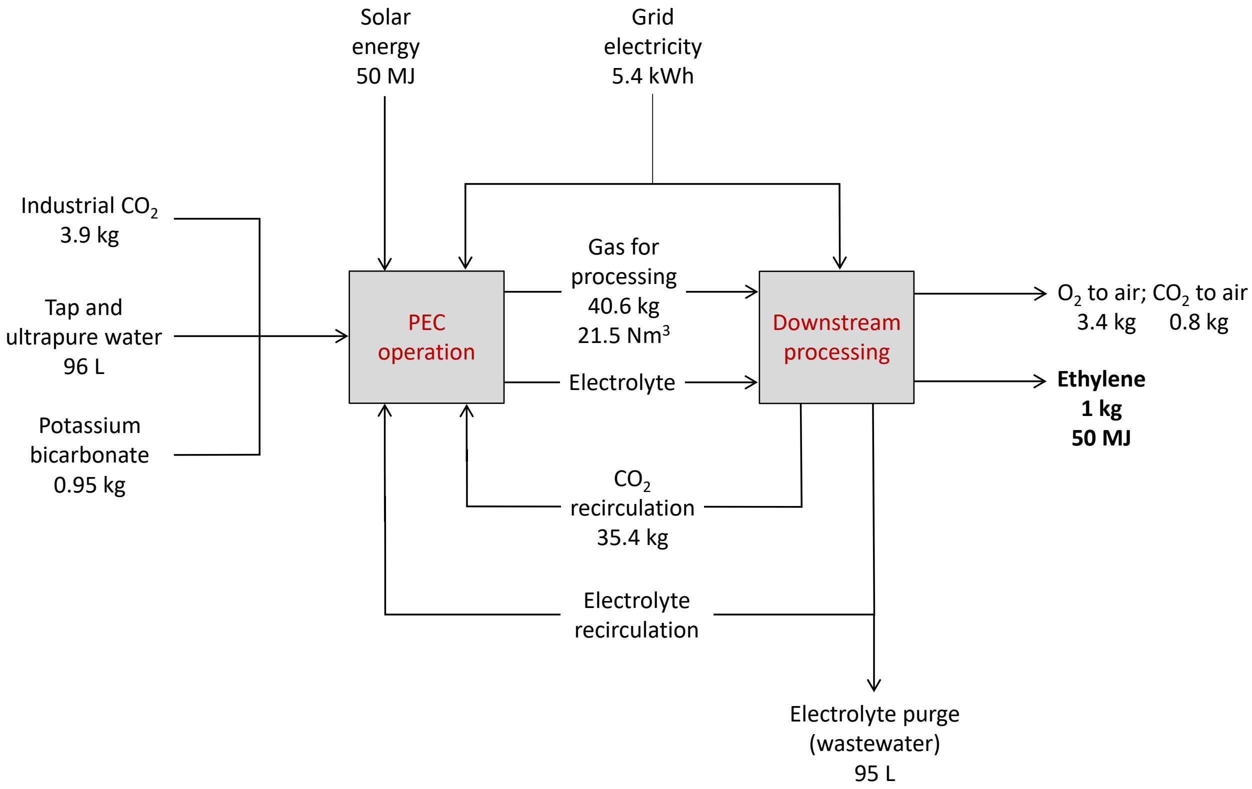

Figure 8. Mass and energy balance for the LICROX plant operation.

In the following sections the inventory for each of the relevant flows in the bullet points above is described, while in section 3.3.8 the inventory for operation as a whole is summarized.

3.3.1 Carbon dioxide supply

The stoichiometric amount of CO_2 needed to produce ethylene, following the chemical reaction in Equation 1, is 3.14 kg/kg ethylene, however the overall CO_2 utilization efficiency by the process, once recirculation of this gas is considered, has been established by the LICROX consortium at 80%. Thus, 3.93 kg CO_2 need to be supplied per kg ethylene produced, of which 3.14 kg are captured in the product and 0.79 kg correspond to losses, which are emitted to the atmosphere.

In this study, carbon dioxide supply is included in three formats:

- Pressurized carbon dioxide, supplied via pipeline: this is pure carbon dioxide and considered as the default supply option to the LICROX plant.
- Flue gas, supplied via pipeline: this corresponds to exhaust gases from a power plant, containing approximately 14% carbon dioxide by mass. This is only considered as an alternative option that the LICROX consortium is interested in exploring.
- Carbon dioxide, liquid: this is pure carbon dioxide in liquid form. This option is considered as the most likely supply format to the industrial production of potassium bicarbonate (see section 3.3.3), but is not considered as a supply format to the LICROX plant. For this data set, an average global scenario is considered, in a similar way as in the production of chemicals used in the manufacturing of the PEC.

In the paragraphs below the data sources and assumptions made in the inventories for carbon dioxide supply are described, while Table 28 shows the actual inventory data for the three supply formats mentioned above. As discussed in section 2.10.1, the use of CO_2 as a raw material prevents its emission to the atmosphere. This is reflected in the inventory in Table 28 as an emission of negative sign.

Table 28. Inventory data for carbon dioxide supply.

Activity	Unit	Carbon dioxide, pressurized {EU}	Carbon dioxide, liquid {GLO}	Carbon dioxide, in flue gas {EU}	Data set used and comments
Outputs: Reference flow					
Carbon dioxide, pressurized {EU}	kg	1			
Carbon dioxide, liquid {GLO}	kg		1		
Carbon dioxide, in flue gas {EU}	kg			1	
Inputs: Products and services					
Plant infrastructure	Unit	4.0E-10		4.0E-10	Chemical factory, organics {RER}| construction | Conseq, U
Plant infrastructure	Unit		4.0E-10		Chemical factory, organics {RoW}| construction | Conseq, U
Monoethanolamine	Kg	0.002	0.002		Monoethanolamine {GLO}| market for | Conseq, U
Electricity	kWh	0.097		0.025	Electricity, medium voltage {RER}| market group for | Conseq, U
Electricity	kWh		0.215		Electricity, medium voltage {GLO}| market group for | Conseq, U
Thermal energy	MJ	3.134			Heat, from steam, in chemical industry {RER}| market for heat, from steam, in chemical industry | Conseq, U
Thermal energy	MJ		3.134		Heat, from steam, in chemical industry {RoW}| steam production, as energy carrier, in chemical industry | Conseq, U
Train transport	tkm		0.031		Transport, freight train {GLO}| market group for | Conseq, U
Road transport	tkm		0.021		Transport, freight, lorry, unspecified {GLO}| market group for transport, freight, lorry, unspecified | Conseq, U
Pipeline	km	1.74E-08		6.23E-11	Pipeline, natural gas, long distance, low capacity, onshore {GLO}| market for | Conseq, U
Outputs: Emissions to air					
Carbon dioxide, fossil	kg	-1	-1	-1	Avoided emission.
Monoethanolamine	kg	0.002	0.002		Monoethanolamine losses

The inventory for carbon dioxide capture from point-source flue gases through amine scrubbing is based on data by Rosental et al. (2020), including the energy (electricity and heat) and monoethanolamine (MEA) consumption by the process, for a plant producing 1.88 million tonne CO_2 per year. The fate of MEA losses is not discussed by the authors and it is assumed here to be lost to the atmosphere, in line with the data set for liquid carbon dioxide production in the ecoinvent database. Infrastructure for the production process is not included by Rosental et al. (2020) either. This is approximated in the study with an input of generic organic chemical facility, as done in the ecoinvent database for production of chemicals.

Transport of the captured carbon dioxide in gaseous form through a pipeline requires pressurization. According to Croezen et al. (2018), the current OCAP-pipeline pressure is standardized at 21 bar. For a doubling of capacity, the pressure will need to be higher, estimated at approximately 40 bar in pressure. The authors assume that the carbon dioxide stream is at 1 bar pressure, where an increase to 40 bar requires 0.295 MJ electricity per kg carbon dioxide. Infrastructure, i.e. pipeline construction and disposal, is not addressed by Croezen et al. (2018), but is addressed in the present study based on the following figures:

- A pipeline length of 347 km (OCAP 2018).
- A pipeline capacity of 500,000 tonne carbon dioxide per year (OCAP 2018).
- An assumed pipeline life span of 50 years, in line with the value assumed for natural gas pipelines in the ecoinvent database.

With the above data, it can be calculated that 1 kg CO_2 requires the construction and disposal of 1.74E-08 km of pipeline. This activity is represented in the model with the global ecoinvent data set for an onshore natural gas pipeline.

Regarding carbon dioxide in liquid form, a data set is available in the ecoinvent database, but it is preferred in the present study to use alternative data as far as possible. The reasons for this are that:

- The data set is rather old, using primary data from the 1990's.
- The inventory includes emissions to air of methane present in the gas stream from where the CO_2 is captured. It can be stated that a demand for liquid CO_2 does not lead to additional methane emissions to the atmosphere, since these would have been emitted anyway. Thus, this data set is not in its present form properly considering a consequential inventory modelling.

The inventory for carbon dioxide supply in liquid form considers, as a first step, the same data for capture with MEA, as described above, based on data from Rosental et al. (2020). Electricity consumption for the subsequent step of carbon dioxide liquefaction is taken as 0.72 MJ/kg CO_2 (Frischknecht et al. 2007). Transport of the liquid CO_2 to the final user is included with the same transport services as in the ecoinvent database.

Regarding carbon dioxide supply in unprocessed flue gas, the inventory only includes an estimate for the pipeline infrastructure and energy consumption for transport. The flue gas is assumed to originate in a natural gas-fired power plant, where the mass fraction of CO_2 is calculated as 14% (see Table 29), based on data from Song et al. (2004).

Table 29. Calculating the mass fraction of carbon dioxide in unprocessed flue gas from a natural gas-fired power plant.

Component in flue gas	% in volume[a]	Density (kg/Nm^3)	Mass by component in flue gas (kg/Nm^3)	Mass by component in flue gas (%)
CO_2	9	1.96	0.177	14%
H_2O	19	0.80	0.153	12%
O_2	3	1.43	0.043	3%
N_2	69	1.25	0.863	70%
Total	100	-	1.235	100%

[a] Data from Song et al. (2004).

The energy consumption and infrastructure requirements for flue gas supply are based on estimates for supply of such flue gases to hypothetical microalgae production plants, where these CO_2-rich gases can be used to boost photosynthetic activity. In such a scenario, to minimize costs, the power plant supplying the gases is assumed to be at a distance of less than 5 km. Electricity consumption for gas transport from a power plant was calculated by Brentner et al. (2011) as 169 MJ/tonne algae, where 1 tonne algae require 1.79 tonne CO_2. This leads to a specific electricity consumption of 0.09 MJ or 0.025 kWh per kg CO_2 supplied. Regarding infrastructure, this was not addressed by Brentner et al. (2011) or in any other LCA of microalgae we have reviewed. It is thus included in the present study with a coarse estimate, based on the following data:

- The transport distance is 2.5 km from power plant to the user. This distance is mentioned by several microalgae studies as the most realistic (Benemann and Oswald 1996; Campbell et al. 2011).
- The CO_2 mass fraction is 14% (Table 29), implying that delivering 1 kg CO_2 requires transporting 7.14 kg flue gas.
- 1 ton-km gas transport requires the construction and disposal of 3.57E-09 km pipeline, based on the ecoinvent data set for transporting natural gas through pipelines in the Netherlands. The value for the Netherlands is taken as a worst case, given that for other countries in the ecoinvent database this figure is lower.

From the above data it can be calculated that the delivery of 1 kg CO_2 requires the construction and disposal of 6.23E-11 km of pipeline. This activity is represented in the model with the global ecoinvent data set for an onshore natural gas pipeline.

3.3.2 Process water

Process water is calculated on a stoichiometric basis, following the chemical reaction in Equation 1. The volume of water required is 1.29 L/kg ethylene. This supply is modelled with the ecoinvent data set for ultrapure water production in Europe by means of electrodeionization. This data set includes not only the operational inputs (chemicals, energy) to process the water, but also an estimate of infrastructure (ion exchanger, membranes, etc.), whereby this aspect does not need to be separately accounted for as part of the plant infrastructure in section 3.2.

3.3.3 Electrolyte production

The electrolyte consists of a 0.1 Molar solution of potassium bicarbonate in pure water. The electrolyte volume per m^2 PEC is 10 L, and it is assumed by the LICROX consortium that this volume needs to be replaced on a weekly basis, even though this is quite uncertain at this stage. The resulting electrolyte consumption per kg ethylene is 95 L, which weights 95.5 kg based on an estimated electrolyte density of 1.005 kg/L. The consumption of potassium bicarbonate and pure water per kg ethylene produced is 0.95 kg and 94.5 L, respectively. Ultrapure water is modelled with the same ecoinvent data set mentioned in section 3.3.2, while potassium bicarbonate, which is not currently covered by the ecoinvent database, is approximated with the inventory data in Table 30, which are described in the paragraphs below.

Table 30. Inventory data for potassium bicarbonate production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Potassium bicarbonate {GLO}	kg	1	
Inputs: Products and services			
Potassium carbonate	kg	0.69	Potassium carbonate {GLO}| market for | Conseq, U
Carbon dioxide	kg	0.22	Carbon dioxide, liquid {GLO} (LCI data in Table 28)
Process water	kg	0.09	Water, decarbonised {RoW}| market for water, decarbonised | Conseq, U
Electricity	kWh	0.323	Electricity, medium voltage {GLO}| market group for | Conseq, U
Infrastructure	kg	4E-10	Chemical factory, organics {GLO}| market for | Conseq, U
Transport of final product	kg	1	Transport, for chemicals {GLO} (LCI data in Table 9)

Potassium bicarbonate, with the formula $KHCO_3$, is manufactured by treating an aqueous solution of potassium carbonate with carbon dioxide, as shown in Equation 11 (Schultz et al. 2005):

$$K_2CO_3 + CO_2 + H_2O \rightarrow 2\ KHCO_3$$

Equation 11. Chemical reaction for production of potassium bicarbonate.

From Equation 11 the stoichiometric amounts of raw materials have been obtained, while other inputs to the production process (energy, infrastructure) are approximated from the ecoinvent data set for production of ammonium bicarbonate. The inventory also includes transport of the final product.

3.3.4 Electricity for auxiliary equipment

Hysytech estimates that power consumption by the LICROX plant, excluding downstream processing, is likely to fall in the range of 0.005-0.006 kW/m^2 PEC. The arithmetic average value of 0.055 kW/m^2 is used in the study. The average operating hours by the plant is established by the consortium as 10 h/day, and the ethylene yield is 0.015 kg/m^2 PEC/day. Under these assumptions, the electricity consumption can be estimated at 3.67 kWh/kg ethylene. This is modelled with the European electricity supply mix at medium voltage in the ecoinvent database.

3.3.5 Tap water

Tap water is used only for cleaning purposes, to keep the cells free of dust. The volume of water is taken from Sathre et al. (2014) as 25 litres/m^2-year, a typical value for photovoltaics. Based on the ethylene yield of 0.015 kg/m^2 PEC/day and assuming the plant is in operation 90% of days in the year (Ibid.), the water consumption is calculated at 5.07 L/kg ethylene. This is modelled with the European tap water supply data set available in the ecoinvent database.

3.3.6 Downstream processing

The processing of ethylene obtained by the PEC device is expected to include a separation and purification process, consisting of a pressure swing adsorption process. The inventory for operation of this unit includes the following items:

- Electricity consumption.
- Generation of spent electrolyte for disposal as wastewater.
- Emissions to air of by-product gases.

Hysytech has provided a preliminary estimate for the electricity consumption of the PSA unit, at 6 MJ/kg ethylene, which is a worst-case figure obtained from the system design by Sen (2020). This is modelled with the European electricity supply mix at medium voltage in the ecoinvent database.

In a steady-state system, the volume of spent electrolyte generated equals the net input, as quantified in section 3.3.3. This corresponds to 95 L or 95.5 kg effluent, assumed to be discharged as urban wastewater. Inventory data for the wastewater management process is described in section 3.3.7.

Finally, the emissions to air taking place at the PSA unit include carbon dioxide losses and oxygen (see Figure 8). As mentioned in section 3.3.1, the net efficiency of CO_2 utilization in the plant has been established at 80% by the LICROX consortium. This means per kg ethylene 0.79 kg CO_2 are lost to the atmosphere. Regarding oxygen, this is quantified on a stoichiometric basis as 3.43 kg per kg ethylene, following the chemical reaction in Equation 1.

The final inventory data for DSP are incorporated as part of the overall inventory for the LICROX plant operation in section 3.3.8, per kg final ethylene produced.

3.3.7 Electrolyte wastewater disposal

It is assumed that the spent electrolyte can be discharged as urban wastewater. The inventory for disposal of this wastewater reflects its management as urban wastewater in an average European scenario, obtained with the WW LCI v.4 model developed by 2.-0 LCA consultants (Muñoz 2021). This model calculates LCIs for urban wastewater taking into account the specific composition of the wastewater defined by the user, in this case containing 10 g potassium bicarbonate and 990 g water per kg. The model includes the entire chain of wastewater management activities (sewer transport, treatment in different types of wastewater treatment plants, treatment and disposal of sludge, wastewater reuse in agriculture) and a database with country-specific statistics on wastewater management, from which an average European scenario can be obtained. In this scenario, 93% of the wastewater is treated, mainly in plants with tertiary treatment, while 7% is discharged without treatment. 4% of the treated wastewater is reused in agriculture, substituting sea water desalination. Sludge disposal is not relevant in this particular inventory, given that potassium bicarbonate passes through the treatment plant unchanged, and for this reason the model does not account for any sludge production. The model links in the background to the ecoinvent database v3.6, which is consistent with this study. The inventory for wastewater treatment, per kg wastewater is shown in Table 31.

Table 31. Inventory data for electrolyte wastewater treatment.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Electrolyte wastewater {EU}	kg	1	
Outputs: Substituted products and services			
Sea water desalination	kg	-4.3E-03	Tap water {GLO}| tap water production, seawater reverse osmosis, ultrafiltration pretreatment, baseline module, single stage | Conseq, U
Groundwater pumping	Unit	-1.4E-08	Pump, 40W {GLO}| market for | Conseq, U
Groundwater pumping	kWh	-3.3E-06	Electricity, medium voltage {Europe without Switzerland}| market group for | Conseq, U
Groundwater pumping	MJ	-5.2E-06	Diesel, burned in building machine {GLO}| market for | Conseq, U
River water	L	-0.016	Substituted river water through wastewater reuse
Groundwater	L	-0.011	Substituted groundwater through wastewater reuse
Inputs: Natural resources			
Occupation, water bodies	m^2yr	1.5E-07	Land occupation by lagoon wastewater treatment plants
Occupation, industrial area	m^2yr	1.9E-07	Land occupation by lagoon wastewater treatment plants
Inputs: Products and services			
Infrastructure	Unit	1.8E-13	Wastewater treatment facility, capacity 4.7E10l/year {GLO}| market for | Conseq, U
Infrastructure	Unit	2.0E-13	Wastewater treatment facility, capacity 1.1E10l/year {GLO}| market for | Conseq, U
Infrastructure	Unit	1.4E-12	Wastewater treatment facility, capacity 5E9l/year {GLO}| market for | Conseq, U
Infrastructure	Unit	3.3E-12	Wastewater treatment facility, capacity 1E9l/year {GLO}| market for | Conseq, U
Infrastructure	Unit	7.4E-12	Wastewater treatment facility, capacity 1.6E8l/year {GLO}| market for | Conseq, U
Infrastructure	km	4.2E-11	Sewer grid, 4.7E10l/year, 583 km {GLO}| market for | Conseq, U
Infrastructure	km	2.0E-11	Sewer grid, 1.1E10l/year, 242 km {GLO}| market for | Conseq, U
Infrastructure	km	6.3E-11	Sewer grid, 5E9l/year, 110 km {GLO}| market for | Conseq, U
Infrastructure	km	4.0E-11	Sewer grid, 1E9l/year, 30 km {GLO}| market for | Conseq, U
Infrastructure	km	1.7E-11	Sewer grid, 1.6E8l/year, 6 km {GLO}| market for | Conseq, U
Infrastructure	m3	1.3E-09	Concrete, normal {RoW}| market for | Conseq, U
Infrastructure	kg	1.2E-07	Reinforcing steel {GLO}| market for | Conseq, U
Infrastructure	kg	1.1E-08	Polyethylene, high density, granulate {GLO}| market for | Conseq, U
Infrastructure	kg	3.2E-09	Polypropylene, granulate {GLO}| market for | Conseq, U
Infrastructure	m3	9.2E-09	Excavation, hydraulic digger {GLO}| market for | Conseq, U
Infrastructure	kg	4.3E-09	Polyvinylchloride, bulk polymerised {GLO}| market for | Conseq, U
Infrastructure	kg	1.8E-08	Extrusion, plastic pipes {GLO}| market for | Conseq, U
Infrastructure	kg	1.1E-05	Sand {RoW}| market for sand | Conseq, U
Infrastructure	kg	3.1E-08	Waste plastic, mixture {Europe without Switzerland}| market group for waste plastic, mixture | Conseq, U
Infrastructure	kg	1.2E-07	Waste reinforcement steel {RoW}| market for waste reinforcement steel | Conseq, U
Infrastructure	kg	1.8E-05	Inert waste, for final disposal {RoW}| market for inert waste, for final disposal | Conseq, U
Infrastructure	kg	2.8E-06	Waste concrete {Europe without Switzerland}| market for waste concrete | Conseq, U
Wastewater treatment	kg	5.0E-06	Sodium hypochlorite, without water, in 15% solution state {RER}| market for sodium hypochlorite, without water, in 15% solution state | Conseq, U
Wastewater treatment	kWh	4.0E-05	Electricity, medium voltage {Europe without Switzerland}| market group for | Conseq, U
Wastewater treatment	MJ	3.2E-05	Heat, district or industrial, natural gas {Europe without Switzerland}| market for heat, district or industrial, natural gas | Conseq, U
Wastewater treatment	kg	5.1E-06	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq, U
Outputs: emissions to water			
Potassium bicarbonate	kg	0.0096	Effluent, treated and untreated, discharged to river/sea
Water	kg	0.959	Effluent, treated and untreated, discharged to river/sea
Outputs: emissions to soil			
Potassium bicarbonate	kg	0.0004	Effluent, reused in agriculture
Water	kg	0.313	Effluent, reused in agriculture

3.3.8 Operation: overall inventory

The overall inventory for the LICROX plant operation is shown in Table 32, building on the items described in section 3.3.1 to 3.3.7. The reference flow is 1 kg ethylene at the outlet of the DSP unit. It can be seen that the inventory includes the amount of solar energy absorbed to produce ethylene. This amount equals the chemical energy stored in ethylene, which is equivalent to its gross calorific value, namely 50.3 MJ/kg (Engineering ToolBox 2003a).

Table 32. Inventory data for LICROX plant operation.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
LICROX plant operation {EU}	kg	1	
Inputs: Natural resources			
Energy, solar, converted	MJ	50.3	
Inputs: Products and services			
Carbon dioxide	kg	3.93	Carbon dioxide, pressurized {EU} (LCI data in Table 28)
Process water	L	1.3	Water, ultrapure {RER}| water production, ultrapure | Conseq, U
Electrolyte water	L	94.5	Water, ultrapure {RER}| water production, ultrapure | Conseq, U
Potassium bicarbonate	Kg	0.95	Potassium bicarbonate {GLO} (LCI data in Table 30)
Electricity, PEC operation	kWh	3.67	Electricity, medium voltage {RER}| market group for | Conseq, U
Electricity, DSP operation	kWh	1.67	Electricity, medium voltage {RER}| market group for | Conseq, U
Tap water	L	5.07	Tap water {RER}| market group for | Conseq, U
Electrolyte wastewater disposal	kg	95.5	Electrolyte wastewater {EU} (LCI data in Table 31)
Outputs: emissions to air			
Oxygen	kg	3.43	From chemical reaction in Equation 1.
Water	kg	0.91	Evaporated cleaning water.
Carbon dioxide, fossil	kg	0.79	Losses, 20% of total input

3.4 LICROX plant disposal

Dismantling of the LICROX plant is included in the model as a generic scenario for disposal through either recycling, landfilling or incineration with energy recovery of the materials in the PEC and infrastructure. The starting point for the inventory is the amounts of materials reported in sections 3.1.5, 3.2.1 and 3.2.2.

3.4.1 Photoelectrochemical cell disposal

Regarding the PEC, the inventory for its disposal includes the device itself plus its packaging materials. The latter are expected to be disposed of as waste during plant construction rather than during plant decommissioning, but they are included as part of decommissioning for simplicity. The estimated PEC weight is 2.7 kg, of which 2.5 kg consists of glass, 0.14 kg is PET and the remaining 0.07 kg are constituted by a wide variety of materials. As a default scenario, it is assumed that the glass sheet can be separately collected and recycled, while the remaining materials are ultimately sent to landfill or incinerated, depending on the local practices where the plant is located. In the model we use for this disposal scenario the average European scenario for disposal of each material. Regarding packaging, as a default scenario it is assumed that cardboard packaging is sent for recycling, while the EPS foam is sent for disposal. The inventory data used are shown in Table 33, per m^2 PEC.

Table 33. Inventory data for PEC disposal.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
PEC disposal {EU}	m^2 PEC	1	
Inputs: Products and services			
PEC - glass recycling	kg	2.50	Waste packaging glass, unsorted {GLO}| market for | Conseq, U
PEC - PET disposal	kg	0.14	Waste polyethylene terephtalate {Europe without Switzerland}| market for waste polyethylene terephtalate | Conseq, U
PEC - other materials disposal	kg	0.07	Inert waste, for final disposal {CH}| market for inert waste, for final disposal | Conseq, U
Packaging – cardboard recycling	kg	0.36	Waste paperboard, unsorted {CH}| treatment of waste paperboard, unsorted, sorting | Conseq, U
Packaging – EPS disposal	kg	0.44	Waste expanded polystyrene {RoW}| market for waste expanded polystyrene | Conseq, U

3.4.2 Photoelectrochemical cell plant infrastructure materials disposal

Regarding infrastructure materials other than the PEC (excluding the DSP unit), the following disposal scenario has been considered in the inventory (Table 34):

- Metallic components (steel and aluminium structures, etc.), including steel for concrete reinforcement, are sent for recycling. Pumps are treated in the model as steel scrap, also sent for recycling. Steel recycling is currently not covered in the ecoinvent database as a waste treatment activity, but as a (constrained) supply of raw material. In order to be able to use this data set to reflect waste management, it needs to be used with a negative sign in the model.
- Plastic components (pipes, tanks, etc.) are sent for disposal. This is covered with the ecoinvent data set for disposal of plastic mixtures in Europe.
- Concrete is sent for disposal in an inert material landfill. The volume of concrete is expressed in mass terms assuming a density of 2,300 kg/m^3.
- Electronics for control units are disaggregated into three fractions, based on their composition in the ecoinvent database: 46% is steel, sent for recycling; 32% is plastics, assumed to be sent for disposal; 14% is printed wiring boards, sent for electronics recycling; 8% is used cable, also sent for recycling. The ecoinvent data sets for steel recycling and plastics disposal are the same mentioned in the previous paragraphs, while for used cable and printed wiring boards specific ecoinvent data sets for these waste fractions are used.

Table 34. Inventory data for LICROX PEC infrastructure disposal.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
LICROX PEC infrastructure disposal {EU}	m^2 PEC-year	1	
Inputs: Products and services			
Steel to recycling	kg	-1.34[a]	Iron scrap, unsorted {GLO}| market for | Conseq, U
Aluminium to recycling	kg	0.214	Aluminium scrap, post-consumer {GLO}| market for | Conseq, U
Plastics to disposal	kg	0.126	Waste plastic, mixture {RER}| market group for waste plastic, mixture | Conseq, U
Concrete to disposal	kg	26	Waste concrete {Europe without Switzerland}| market for waste concrete | Conseq, U
Printed wiring boards to recycling	kg	0.0046	Used printed wiring boards {GLO}| market for | Conseq, U
Used cable to recycling	kg	0.0026	Used cable {GLO}| market for | Conseq, U

[a] A negative sign is needed for the ecoinvent data set to reflect steel as waste for treatment instead of as a raw material.

3.4.3 Downstream processing plant infrastructure materials disposal

The approach to define the disposal of materials present in the DSP unit infrastructure is similar to that mentioned in the previous section. The starting point is the type and amounts of materials included in the construction inventory, and the definition of a disposal route, also in line with the previous section. The following assumptions have been made:

- Gravel and aluminium oxide are considered to be sent for disposal.
- Concrete waste is sent to landfill. The volume of concrete is expressed in mass units by means of a density of 2,370 kg/m^3, the value for normal concrete considered in the ecoinvent database.
- Machinery (pump, chiller, compressor, expansion vessel) is characterized in the model together with steel scrap, sent for recycling. The weight of machinery in kg is calculated based on the unitary weights reported in the meta-data of the corresponding ecoinvent data sets for production of each piece of equipment.
- Brass is assumed to be sent for recycling, but there are no data sets for brass waste in the ecoinvent database. Recycling of copper waste is used as an approximation.

Following the approach taken for reporting the inventory data for DSP infrastructure construction, the reference flow in the final disposal stage of this infrastructure is also 1 Nm^3 processed gas, as shown in Table 35.

Table 35. Inventory data for LICROX DSP infrastructure disposal.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
LICROX DSP infrastructure disposal {EU}	Nm^3 gas input	1	1 Nm^3 gas input to the PSA unit
Inputs: Products and services			
Steel to recycling	kg	-5.99E-04[a]	Iron scrap, unsorted {GLO}| market for | Conseq, U
Wastewater to disposal	Litres	2.40E-05	Wastewater, unpolluted {RoW}| market for wastewater, unpolluted | Conseq, U
Glycol to disposal	kg	1.15E-05	Spent antifreezer liquid {GLO}| market for | Conseq, U
Mineral oil to disposal	kg	7.71E-06	Waste mineral oil {Europe without Switzerland}| treatment of waste mineral oil, hazardous waste incineration | Conseq, U
Gravel and aluminium oxide to disposal	kg	7.81E-04	Inert waste {Europe without Switzerland}| market for inert waste | Conseq, U
Concrete to disposal	kg	8.33E-04	Waste concrete {Europe without Switzerland}| market for waste concrete | Conseq, U
Brass to recycling	kg	6.42E-09	Copper scrap, sorted, pressed {GLO}| market for | Conseq, U
Polypropylene to disposal	kg	4.14E-05	Waste polypropylene {RER}| market group for waste polypropylene | Conseq, U
Aluminium to recycling	kg	4.71E-09	Aluminium scrap, post-consumer {GLO}| market for | Conseq, U

[a] A negative sign is needed for the ecoinvent data set to reflect steel as waste for treatment instead of as a raw material.

3.5 LICROX: overall inventory

Table 36 shows the final inventory for production of 1 kg ethylene by the LICROX plant. The table links to the respective, previously described, inventories for PEC production, infrastructure production, plant operation, PEC disposal and infrastructure disposal. The only underlying activity where the reference flow is

1 kg ethylene is the LICROX plant operation, while all other activities have different reference flows. For PEC production and PEC infrastructure, the reference flow is PEC area (m^2) and PEC area-time (m^2 PEC-year), respectively. For DSP infrastructure, the reference flow is the volume of unprocessed gases entering the process (in Nm^3).

These activities can be expressed per functional unit (1 kg ethylene) as follows:

- According to the LICROX consortium, the expected service life of the PEC device is 10 years. Based on a yield of 0.015 kg ethylene/m^2 PEC-day and assuming the plant operates 90% of the time (Sathre et al. 2014) 365 days/year, 1 m^2 PEC is expected to produce a total of 49.275 kg ethylene during its service life. Thus, 1 kg ethylene can be attributed the replacement of 1/49.275 = 0.0203 m^2 PEC.
- PEC Infrastructure activities are expressed per m^2 PEC-year. Based on the above-mentioned yield of 0.015 kg ethylene/m^2 PEC-day, 1 m^2 PEC-year is associated with the production of 4.9275 kg ethylene. Thus, 1 kg ethylene can be attributed 1/4.9275 = 0.203 m^2 PEC-year worth of plant infrastructure.
- DSP infrastructure activities are expressed per Nm^3 unprocessed gas entering the pressure swing adsorption process. This has been quantified in the mass balance (Figure 8) as 21.5 Nm^3 gas per kg ethylene.

Table 36. Inventory data for ethylene production by the LICROX plant.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Ethylene, LICROX {EU}	kg	1	
Inputs: Products and services			
PEC production	m^2 PEC	0.0203	PEC, $BiVO_4$ {EU} (LCI data in Table 6)
PEC infrastructure	m^2 PEC-year	0.203	LICROX PEC infrastructure {EU} (LCI data in Table 24)
DSP infrastructure	Nm^3 gas input	21.5	LICROX DSP infrastructure {EU} (LCI data in Table 25)
Plant operation	kg	1	LICROX plant operation {EU} (LCI data in Table 32)
PEC disposal	m^2 PEC	0.0203	PEC disposal {EU} (LCI data in Table 33)
PEC infrastructure disposal	m^2 PEC-year	0.203	LICROX plant infrastructure disposal {EU} (LCI data in Table 34)
DSP infrastructure disposal	Nm^3 gas input	21.5	LICROX DSP infrastructure disposal {EU} (LCI data in Table 35)

3.6 Steam cracking

3.6.1 Ethylene production

Inventory data for ethylene production by steam cracking of naphtha are shown in Table 37. The data are based on the mass and energy balance provided by Rodríguez-Vallejo et al. (2020), which is in turn based on the work by Yang and You (2017). The authors provide the data using 1 kg propylene as reference flow. This is changed in Table 37, where the reference flow is instead the determining product of this process, namely ethylene.

Table 37. Inventory data for ethylene production by steam cracking.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Ethylene, petrochemical {EU}	kg	1	
Outputs: By-products			
Propylene	kg	-0.410	Propylene, petrochemical {EU} (LCI data in Table 38)
C4 hydrocarbons, as butadiene	kg	-0.057	Butadiene {RER}| market for butadiene | Conseq, U
C5+ hydrocarbons, as naphtha	kg	-1.074	Naphtha {RER}| market for | Conseq, U
Inputs: Products and services			
iLUC, arable land	kg NPP_0 as C	9.45E-05	Arable land, as NPP0 {GLO} (LCI data in Table 27)
Naphtha	kg	2.94	Naphtha {RER}| market for | Conseq, U
Sodium hydroxide	kg	4.75E-04	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq, U
Electricity	kWh	0.743	Electricity, medium voltage {RER}| market group for | Conseq, U
Steam	MJ	3.619	Heat, from steam, in chemical industry {RER}| market for heat, from steam, in chemical industry | Conseq, U
Cooling energy	MJ	0.014	Cooling energy {EU} (LCI data in Table 39)
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| market for | Conseq, U
Outputs: Emissions to air			
Carbon dioxide, fossil	kg	1.311	
Carbon monoxide, fossil	kg	3.51E-04	
Mercury	kg	3.25E-08	
Methane, fossil	kg	1.16E-04	
Nitrogen oxides	kg	0.00105	
NMVOC	kg	1.16E-04	
Particulates, < 2.5 um	kg	1.28E-04	
Radon-222	kBq	0.149	
Sulfur dioxide	kg	0.00065	

The process according to Rodríguez-Vallejo et al. (2020) obtains three by-products: propylene, C4 hydrocarbons and C5+ hydrocarbons. For propylene, a dedicated inventory is provided in section 3.6.2. The other two by-products are included in the model as follows:

- According to Jukić (2013) C4 hydrocarbons produced by steam cracking are a mixture where the main component is butadiene. This by-product is then included in the model as a butadiene by-product.
- C5+ hydrocarbons are a mixture of hydrocarbons with 5 or more carbon atoms. According to Jukić (2013), this flow corresponds to pyrolysis gasoline, also known as Pygas, which is the third largest by-product, in mass terms, from steam cracking. Pyrolysis gasoline is a naphtha range intermediate, used for aromatics production or in gasoline blending. In the inventory, this by-product is considered to substitute an equivalent mass of naphtha.

Regarding energy use, Rodríguez-Vallejo et al. (2020) reports on the use of electricity, steam and cooling energy. Both electricity and steam are included in the model with existing ecoinvent data sets, while for cooling, a specific data set has been produced for this study, as described in section 3.6.3.

Rodríguez-Vallejo et al. (2020) only reported direct emissions to air of CO_2 in the steam cracker, which are included in our model, namely 1.311 kg CO_2 per kg ethylene. This, however, most likely constitutes an incomplete inventory for air emissions from the steam cracker. In order to account for emissions of other pollutants to air, these have been estimated taking the same profile of air emissions as in the ecoinvent data set for heat supply from combustion of refinery gas in Europe. As an example, in this data set it is reported that 1.5E-05 kg CO are emitted for each 0.0561 kg CO_2. In our model, the CO emission is linearly scaled up to 3.51E-04 kg for an emission of 1.311 kg CO_2. The same linear scale-up is performed for seven other emission flows reported in the ecoinvent data set. Even if this estimate involves substantial uncertainty, it is judged to better reflect reality than neglecting emissions altogether.

Besides the data from Rodríguez-Vallejo et al. (2020), an attempt has been made to include in the inventory iLUC effects, in coherence with the LICROX technology, where this is also included. For a steam cracker, the only data found on land occupation by such facilities is related to BASF's Ludwigshafen steam cracker number 2 in Germany, with an area of 64,000 m^2 (BASF 2022) and an ethylene production capacity of 400,000 tonne/year (Petrochemicals Europe 2022). This leads to an occupation of 0.00016 m^2-year/kg ethylene. Considering the arable land NPP_0 value of 591 g carbon/m^2-year in Europe (Table 26), the iLUC flow obtained is 9.45E-05 kg carbon/kg ethylene.

The data by Rodríguez-Vallejo et al. (2020) did not report on infrastructure. This is included in the model with the data set for construction (and disposal) of a factory for production of organic chemicals, used by default in the ecoinvent database, quantified at 4E-10 factory units per kg product.

3.6.2 Propylene production

Steam cracking constitutes the main production route for propylene production globally, and this is reflected in the available data set for this chemical in the ecoinvent database. However, propylene constitutes a by-product from steam cracking, meaning that this technology is not likely to respond to changes in demand for propylene, but to changes in demand for ethylene. Thus, in our steam cracking model, as summarised in Table 37, it would be inconsistent to use the propylene data set from the ecoinvent database, as this implies considering that co-producing propylene by steam cracking substitutes propylene also produced by steam cracking. It is therefore necessary for consistency reasons to elaborate an inventory that reflects the marginal technology – that is, the one responding to changes in demand – for propylene production in Europe.

There are several technologies, besides steam cracking, to produce propylene. These include:

- Fluid catalytic cracking (FCC)
- Propane dehydrogenation
- Methanol-to-propylene (MTP)

FCC constitutes the second largest global supplier of propylene, after steam cracking (Rothaemel and Holtmann 2002), but it cannot be considered as a marginal technology since its determining product is motor gasoline and not propylene. Regarding propane dehydrogenation, this technology is also discarded as marginal technology since its feedstock, propane, is also a by-product from natural gas and crude oil processing. MTP, on the other hand, is flexible to changes in demand for propylene, since the latter is its determining product, and because methanol as feedstock is not constrained. This technology exists at the commercial scale, see for example the 'MegaMethanol' technology by Lurgi (Koempel and Liebner 2007).

Methanol can in turn be produced either via reforming of natural gas or from coal-based coke oven gas. In this study, methanol is assumed to be produced from natural gas, as this is a more likely scenario in Europe. This is aligned with the data set for methanol production in the ecoinvent database, which is used in our model.

Inventory data for propylene production from methanol are shown in Table 38, based on the mass and energy balance provided by Rodríguez-Vallejo et al. (2020), which is the same data source for steam cracking. The primary data included inputs of feedstock (methanol) and energy (steam, cooling), as well as wastewater and the by-products naphtha, ethylene and surplus electricity. Ethylene is included in the model with the same data for steam cracking shown in Table 37. Infrastructure and iLUC effects are included in this inventory using the same approximations as for ethylene from steam cracking.

Table 38. Inventory data for propylene production.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Propylene, petrochemical {EU}	kg	1	
Outputs: By-products			
Ethylene	kg	-0.08	Ethylene, petrochemical {EU} (LCI data in Table 37)
Naphtha	kg	-1.08	Naphtha {RER}| market for | Conseq, U
Electricity	kWh	-0.0114	Electricity, medium voltage {RER}| market group for | Conseq, U
Inputs: Products and services			
iLUC, arable land	kg NPP$_0$ as C	9.45E-05	Arable land, as NPP0 {GLO} (LCI data in Table 27)
Methanol	kg	4.93	Methanol {GLO}| market for | Conseq, U
Electricity	kWh	0.743	Electricity, medium voltage {RER}| market group for | Conseq, U
Steam	MJ	3.67	Heat, from steam, in chemical industry {RER}| market for heat, from steam, in chemical industry | Conseq, U
Cooling energy	MJ	9.49	Cooling energy {EU} (LCI data in Table 39)
Infrastructure	Unit	4.0E-10	Chemical factory, organics {GLO}| market for | Conseq, U
Wastewater treatment	L	2.77	Wastewater, average {Europe without Switzerland}| market for wastewater, average | Conseq, U

3.6.3 Cooling energy

Cooling is a service used by petrochemical ethylene and propylene production. The ecoinvent database includes a data set for cooling energy, where this energy is supplied by an absorption chiller operated with heat from a natural gas cogeneration unit. In a big petrochemical compound, however, cooling is most likely expected to be supplied by cooling towers, but this type of service is not covered as such by the ecoinvent database. In this section an inventory is provided for this service.

The inventory includes the full life cycle of a cooling tower, based on data by Schulze et al. (2019). Tower materials include steel, polyvinylchloride (PVC) and pumps. Processing of steel and plastics to finished components is added by average processes in ecoinvent for metal products and plastic extrusion. Pumps are included as an electric motor, also available in ecoinvent. The end-of-life stage is also included, assuming recycling of steel and pumps and disposal of PVC.

Operation of the cooling tower includes inputs of water and electricity, and an output of wastewater. The difference between input and output water is reflected in the inventory as evaporation. Input water is modelled as softened water, while the output is modelled as unpolluted wastewater.

The service of cooling as such is not determined by Schulze et al. (2019). We have estimated this service in MJ based on the volume of water evaporated during the cooling water service life, multiplied by 2.26, which is the latent heat of vaporization for water, in MJ/kg.

Table 39. Inventory data for cooling energy.

Exchange	Unit	Amount	Data set used and comments
Outputs: Reference flow			
Cooling energy {EU}	MJ	96,036,438	
Inputs: Products and services			
Steel	kg	850	Steel, chromium steel 18/8 {GLO}| market for | Conseq, U
PVC	kg	192.3	Polyvinylchloride, suspension polymerised {GLO}| market for | Conseq, U
Pumps	kg	735	Electric motor, vehicle {GLO}| market for | Conseq, U
PVC components manufacturing	kg	192.3	Extrusion, plastic pipes {GLO}| market for | Conseq, U
Steel components manufacturing	kg	850	Metal working, average for metal product manufacturing {GLO}| market for | Conseq, U
Electricity	MWh	864	Electricity, medium voltage {RER}| market group for | Conseq, U
Water	kg	63,740,000	Water, completely softened {RER}| market for water, completely softened | Conseq, U
Wastewater treatment	L	21,246,001	Wastewater, unpolluted {CH}| market for wastewater, unpolluted | Conseq, U
Steel and pumps to recycling	kg	-1,585[a]	Iron scrap, unsorted {GLO}| market for | Conseq, U
PVC to disposal	kg	192.3	Waste polyvinylchloride {RER}| market group for waste polyvinylchloride | Conseq, U
Outputs: emissions to air			
Water	kg	850	Steel, chromium steel 18/8 {GLO}| market for | Conseq, U

[a] A negative sign is needed for the ecoinvent data set to reflect steel as waste for treatment instead of as a raw material.

4 Life cycle impact assessment and interpretation

4.1 Impact assessment results: mid-point

Table 40 below shows the impact assessment results for ethylene production by steam cracking and by LICROX, using Stepwise at mid-point level, where each impact indicator is expressed in its own units. Figure 9 in turn shows the same results in relative units, where for each indicator, the option with the highest impact (LICROX/steam cracking) is set to 100%, and the other option as the corresponding percentage.

Table 40.Impact assessment results at mid-point level.

Indicator	Unit	Steam cracking	LICROX
Human toxicity, carcinogens	kg C_2H_3Cl-eq	-0.226	0.222
Human toxicity, non-carcinogens	kg C_2H_3Cl-eq	-0.006	0.396
Respiratory inorganics	kg $PM_{2.5}$-eq	0.003	0.015
Ionizing radiation	Bq C-14 into air	84	121
Ozone layer depletion	kg CFC11-eq	1.01E-06	5.09E-07
Ecotoxicity, aquatic	kg TEG-eq into water	36	2383
Ecotoxicity, terrestrial	kg TEG-eq into soil	9	96
Nature occupation	PDF·m^2·yr	-0.002	0.001
Global warming	kg CO_2-eq	0.16	5.39
Acidification	m^2 UES	0.14	0.68
Eutrophication, aquatic	kg NO_3-eq	-0.0005	0.09
Eutrophication, terrestrial	m^2 UES	0.130	0.96
Respiratory organics	Person·ppm·h	-0.0002	0.0058
Photochemical ozone, vegetation	m^2·ppm·h	1	61
Non-renewable energy demand	MJ primary	33	146
Mineral extraction	MJ extra	0.05	0.91

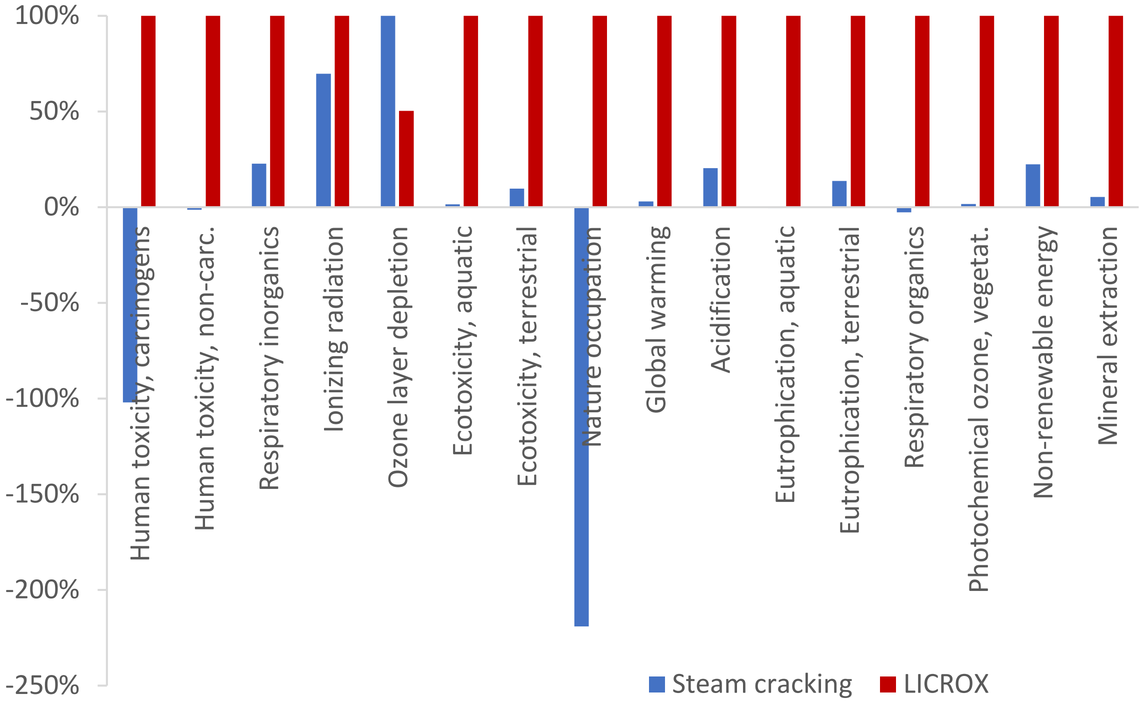

Figure 9. Impact assessment results at mid-point level, in relative units. In each indicator, the highest-score is set to 100%.

The results show, as a general pattern, a higher impact for ethylene produced by LICROX. This is the case for 15 out of the 16 indicators included in Stepwise. As an example, the global warming impact of LICROX is 34 times that of steam cracking, and the non-renewable energy demand 4 times higher than that of steam cracking. In some cases, most notably in nature occupation, LICROX involves an environmental impact (a score of positive sign), while steam cracking involves an environmental saving or credit (a score of negative sign). Results are only favourable for LICROX in the indicator for ozone layer depletion, where the LICROX score is 50% lower than for steam cracking.

In the next section the impact assessment results are expressed after weighting for monetary value, in order to rank all indicators by relevance.

4.2 Impact assessment results: monetarisation

Table 41 below shows the impact assessment results, weighted for monetary value according to the Stepwise method. All indicators are expressed in EUR_{2003}. These results are also graphically shown in Figure 10.

Table 41.Impact assessment results at end-point level.

Indicator	Unit	Steam cracking	LICROX
Respiratory inorganics	EUR_{2003}	0.235	1.037
Global warming	EUR_{2003}	0.013	0.448
Human toxicity, non-carc.	EUR_{2003}	-0.002	0.107
Ecotoxicity, terrestrial	EUR_{2003}	0.010	0.106
Human toxicity, carc.	EUR_{2003}	-0.060	0.058
Photochemical ozone	EUR_{2003}	3.8E-04	0.023
Ecotoxicity, aquatic	EUR_{2003}	2.7E-04	0.018
Eutrophication, terrestrial	EUR_{2003}	0.002	0.012
Eutrophication, aquatic	EUR_{2003}	-5.4E-05	0.009
Acidification	EUR_{2003}	0.001	0.005
Mineral extraction	EUR_{2003}	2.0E-04	0.004
Ionizing radiation	EUR_{2003}	0.002	0.002
Respiratory organics	EUR_{2003}	-4.3E-05	0.002
Nature occupation	EUR_{2003}	-3.0E-04	1.4E-04
Ozone layer depletion	EUR_{2003}	1.0E-04	5.3E-05

It can be seen in Figure 10 that most of the environmental damage associated to LICROX, when expressed in monetary units, is associated to two indicators: respiratory inorganics (emissions of particulate pollution) and global warming (emissions of greenhouse gases). In the case of steam cracking, respiratory inorganics causes most of the damage. The contribution by the remaining indicators is relatively low in both systems.

In respiratory inorganics, the environmental impact of LICROX is 5 times higher than for steam cracking, while in global warming it is 34 times higher. In the following sections we provide a detailed contribution analysis in order to understand which are the main reasons explaining the results in these indicators.

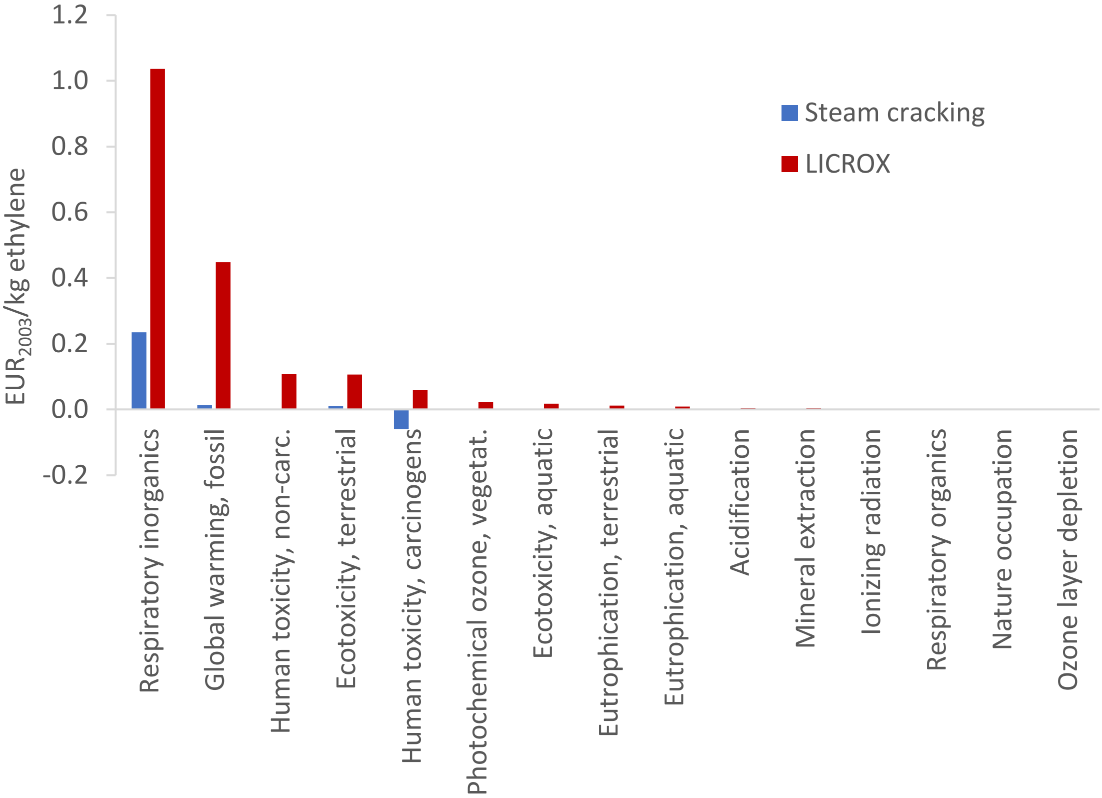

Figure 10. Impact assessment results at end-point level.

4.3 Contribution analysis: respiratory inorganics

4.3.1 Steam cracking

Even though the focus of this study is the LICROX technology, we provide in this section a contribution analysis for ethylene from steam cracking, in order to better understand why its environmental impact is lower than that of LICROX ethylene. Figure 11 shows a breakdown of $PM_{2.5}$-eq emissions associated to ethylene from steam cracking. It shows the total emissions, plus the following contributing activities:

- Direct emissions from the steam cracker.
- Supply of naphtha as raw material for the steam cracker.
- Steam cracker energy use: includes production of electricity and thermal energy to operate the steam cracker.
- Other activities: includes those activities showing an individually minor contribution to the impact, such as iLUC, plant infrastructure, etc.
- Propylene by-product: includes the emissions associated to substituted propylene produced from methanol.
- C4 by-products: includes the emissions associated to substituted butadiene.
- C5 by-products: includes the emissions associated to substituted pyrolysis gasoline.

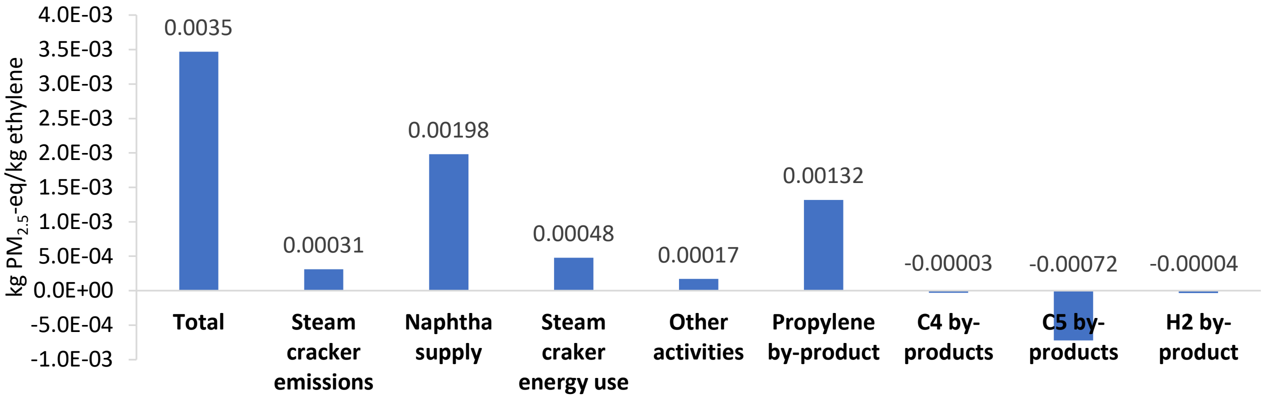

Figure 11. Contribution analysis for steam cracking in the indicator of respiratory inorganics.

Figure 11 shows that the main contribution to respiratory inorganics for steam cracking is the supply of naphtha by a petrochemical refinery. This includes the entire supply chain for production of naphtha, starting at crude oil extraction.

The second most important contribution is the substituted propylene produced from methanol. Since propylene is a by-product, this contribution with a positive sign means that producing propylene from methanol leads to a particulate emission saving. Thus, substituting propylene has the opposite effect, that is, a net particulate emission, as can be seen in Figure 11. A contribution analysis on propylene (not shown here) shows that methanol used as raw material for propylene production involves an emission saving, associated to thermal energy supply from natural gas.

The other by-products, namely C4 hydrocarbons, C5 hydrocarbons and hydrogen lead to a net emission saving, with C5 hydrocarbons constituting the highest saving as it is co-produced in substantially higher quantities than C4 hydrocarbons and hydrogen.

Another relevant contribution appears to be energy consumption by the steam cracker. This consists of electricity and steam. Approximately 36% of this contribution is related to supply of steam, while 64% is related to electricity supply.

4.3.2 LICROX

Figure 12 shows the contribution analysis for ethylene production by the LICROX technology, showing the total emissions and a breakdown by the following activities:

- Land use: includes the iLUC effects associated to the demand for land to build the plant.
- PEC production: includes all activities involved in the supply chain of PEC production, from the production of the raw materials and components to manufacturing of the PEC.
- Plant infra: includes the production of all components and materials used in the plant, other than the PEC. This includes concrete, supporting structures, piping, etc., including the DSP infrastructure.

- Plant operation: includes all material and energy inputs required to operate the LICROX plant (chemicals, water, electricity) including the DSP.
- PEC disposal: includes the disposal by recycling/landfilling/incineration of the PEC.
- Plant infra disposal: includes the disposal by recycling/landfilling/incineration of the other plant infrastructure materials, including those from the DSP.

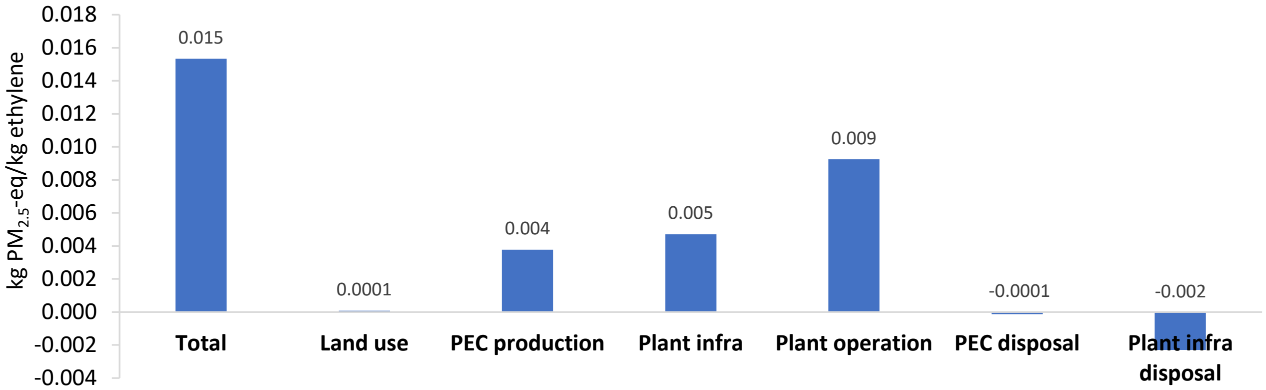

Figure 12. Contribution analysis for LICROX in the indicator of respiratory inorganics.

In Figure 12 it can be seen that, on the one hand, there are several ‘hotspots’ in the life cycle. The main one is plant operation. This life cycle stage contributes with 60% of the particulate emissions. The second most important aspect in the life cycle is the production of the PEC, with 25% of the total particulate emissions. The contribution by plant infrastructure is actually higher than that of PEC production, with 31% of the particulate emissions, however this is partly offset by avoided emissions associated to the infrastructure dismantling, where part of the materials is recycled, leading to the substitution of primary materials. The remaining activities shown in Figure 12 have a minor relevance.

Figure 13 further explores the impact of LICROX plant operation in the indicator of respiratory inorganics, in order to better understand what is driving its remarkable influence in the life cycle. Figure 13 shows the total particulate emissions by this life cycle stage, followed by a breakdown with the following individual activities:

- CO_2 supply: includes the recovery of CO_2 for industrial purposes and its supply to the LICROX plant.
- Water supply: includes production of ultrapure water and tap water, for electrolyte and cleaning purposes, respectively.
- $KHCO_3$ supply: includes production and supply of potassium bicarbonate for electrolyte preparation.
- Electricity, PEC: includes the production of electricity to operate the LICROX plant, excluding downstream processing.
- Electricity, DSPC: includes the production of electricity to operate the downstream processing unit.
- CO_2 losses: direct emissions of CO_2 as a result of losses by the plant. This activity is only relevant when addressing the indicator of global warming.
- Electrolyte wastewater: includes the disposal of electrolyte wastewater.

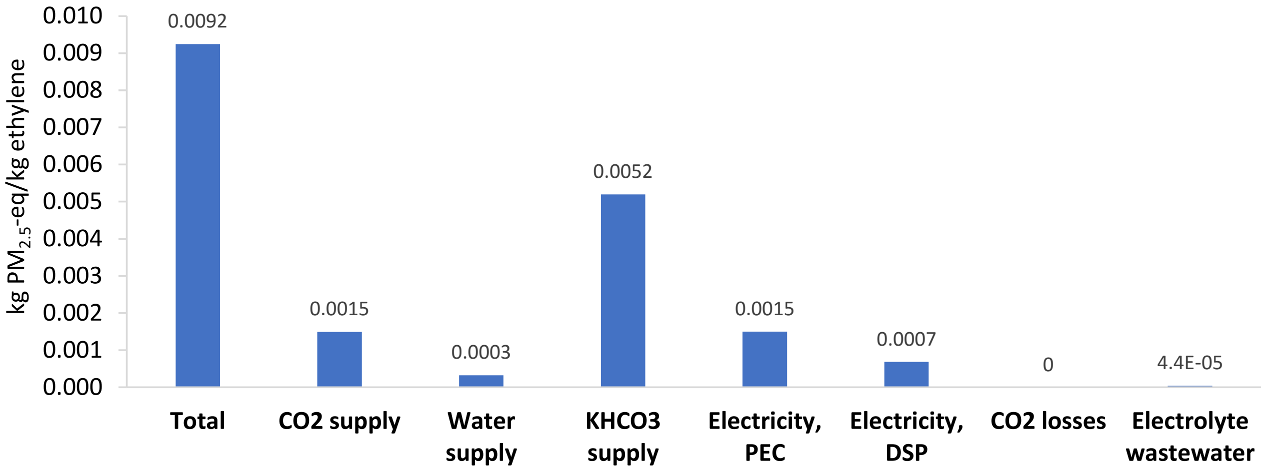

Figure 13. Contribution analysis for LICROX operation in the indicator of respiratory inorganics.

In Figure 13 it can be seen that the most important single aspect explaining the impact of LICROX plant operation is the supply of potassium bicarbonate, used in the PEC electrolyte. The preparation of the electrolyte is also the main water-consuming activity. If the two contributions are added ($KHCO_3$ supply plus water supply), it turns out that electrolyte preparation is responsible for 60% of the plant operation's impact on particulate pollution emissions. It must be highlighted that as a default scenario, the volume of electrolyte is expected to be replaced on a weekly basis, resulting in a specific consumption of 0.95 kg potassium bicarbonate per kg ethylene produced, together with 94.5 L ultrapure water.

The second most important contribution in Figure 13 is electricity supply. It has been estimated that the plant consumes 5.4 kWh/kg ethylene, with 69% of this associated to PEC operation and 31% to the DSP unit. These activities combined represent 24% of the total particulate emissions associated to plant operation as a life cycle stage.

Supply of CO_2 as a reagent contributes with 16% of the total particulate emissions associated to plant operation. Finally, electrolyte wastewater disposal appears to have a relatively low contribution.

4.4 Contribution analysis: global warming

4.4.1 Steam cracking

In this section we provide a detailed contribution analysis for ethylene from steam cracking in the global warming indicator, in order to better understand why its environmental impact is lower than that of LICROX ethylene. Figure 14 shows a breakdown of CO_2-eq emissions associated to ethylene from steam cracking. It shows the total emissions, plus the contribution of the same activities mentioned in section 4.3.1

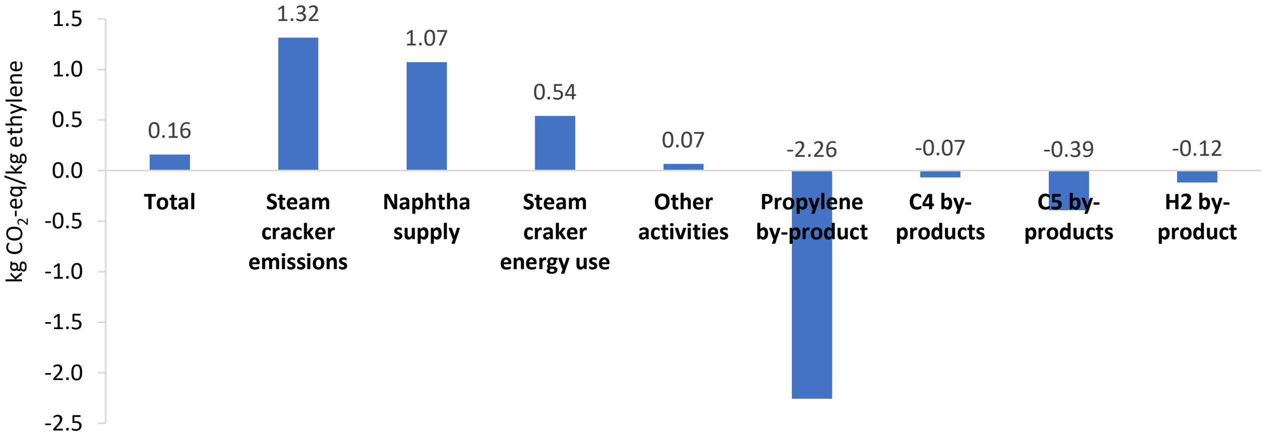

Figure 14. Contribution analysis for steam cracking in the indicator of global warming.

As in the indicator of respiratory inorganics, global warming also shows contributions of positive (impacts) and negative (savings) signs. On the one hand, the largest single contribution to GHG impacts are the direct emissions of CO_2 generated in the steam cracker. This is closely followed by the supply of naphtha as raw material. Supply of energy in the form of steam and electricity is the third most important contributor to the global warming impact. Although not shown in Figure 14, 30% of the contribution is associated to electricity supply and 70% to steam supply. On the other hand, the four types of by-products offset a substantial part of the above-mentioned emissions, as they substitute various products in the market. Most of this offset, shown Figure 14 as values with a negative sign, correspond to propylene. The marginal technology for propylene production (conversion from methanol) leads to a CO_2-eq footprint of 5.5 kg CO_2-eq per kg propylene. Given that 1 kg ethylene co-produces 0.41 kg propylene, this results in a GHG emission saving of 2.26 kg CO_2-eq/kg ethylene. Besides propylene, C4 and C5 hydrocarbons as well as hydrogen also leads to a GHG emission saving, although in all cases of much lower magnitude. Overall, the induced GHG emissions by ethylene production are just slightly higher than those avoided, resulting in a rather low footprint of 0.16 kg CO_2-eq/kg ethylene.

4.4.2 LICROX

Figure 15 shows the contribution analysis for ethylene production by the LICROX technology, showing the total GHG emissions and a breakdown by the same activities mentioned in section 4.3.2.

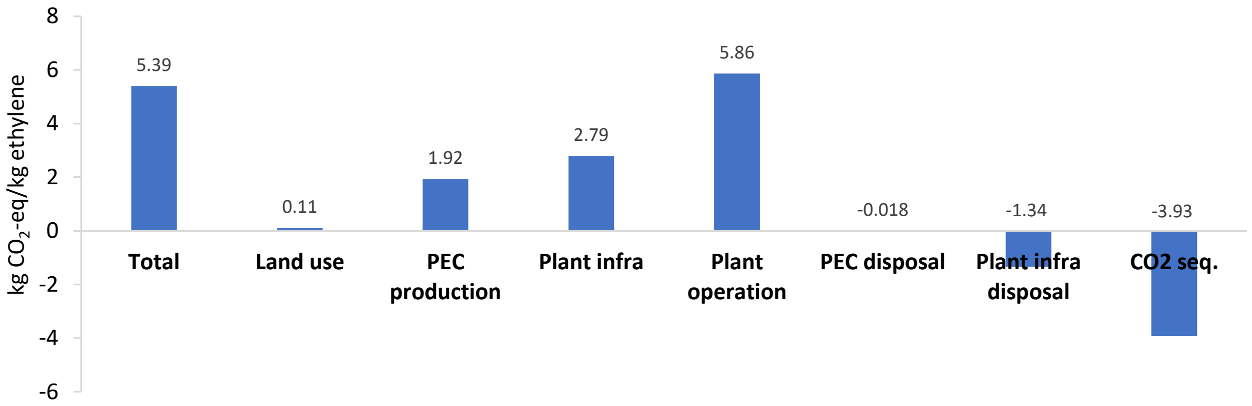

Figure 15. Contribution analysis for LICROX in the indicator of global warming.

In Figure 15 it can be seen that, as in the indicator of respiratory inorganics, there is on the one hand a clear 'hotspot' in the life cycle, and this is plant operation. If contributions with a negative sign are excluded, this life cycle stage can be interpreted to be responsible of 55% of the total GHG emissions. On the other hand, it can also be seen that LICROX involves an avoided emission of -3.93 kg CO_2-eq per kg ethylene. This is the amount of CO_2 supplied to the plant per kg ethylene produced, which would have otherwise been emitted to the atmosphere. In reality, the net amount of CO_2 sequestered in ethylene molecules is 3.14 kg, since the remaining 0.79 kg CO_2 are in fact lost to the atmosphere by the plant. These CO_2 losses are accounted for under the 'Plant operation' contribution in Figure 15 (see Figure 16 for a breakdown of plant operation GHG emissions). This sequestration of CO_2 is a key benefit of the LICROX technology when compared to petrochemical ethylene.

It can also be highlighted the contribution by PEC production. Even though the study assumes the devices will last for 10 years, they still are responsible for 36% of the net GHG emissions. The life cycle GHG emissions of PEC production, from cradle to gate, correspond to 95 kg CO_2-eq/m^2 PEC, where 80% of these emissions are associated to electricity consumption. This GHG footprint is, for example, lower than the 240 kg CO_2-eq/m^2 for a multicrystalline silicon photovoltaic panel produced in Europe according to the ecoinvent database, however photovoltaic panels are expected to last 30 years. This means that on an annual basis, the cradle to gate GHG footprint per m^2 for PEC and photovoltaic panels is approximately in the same order of magnitude.

The contribution by plant infrastructure is actually higher than that of PEC production, being responsible for 52% of the GHG emissions, however this is partly offset by the substitution of primary raw materials resulting from the recycling/energy recovery associated to plant dismantling.

Comparatively, all other aspects in the life cycle show a low or even negligible contribution. The contribution by iLUC ('land use' in Figure 15) is rather low, in spite of LICROX being a potentially land-demanding activity.

Figure 16 further explores the impact of LICROX plant operation in the indicator of global warming, in order to better understand what is driving its substantial influence in the life cycle. Figure 16 shows the total CO_2-

eq emissions by this life cycle stage, followed by a breakdown with the same individual activities mentioned in section 4.3.2.

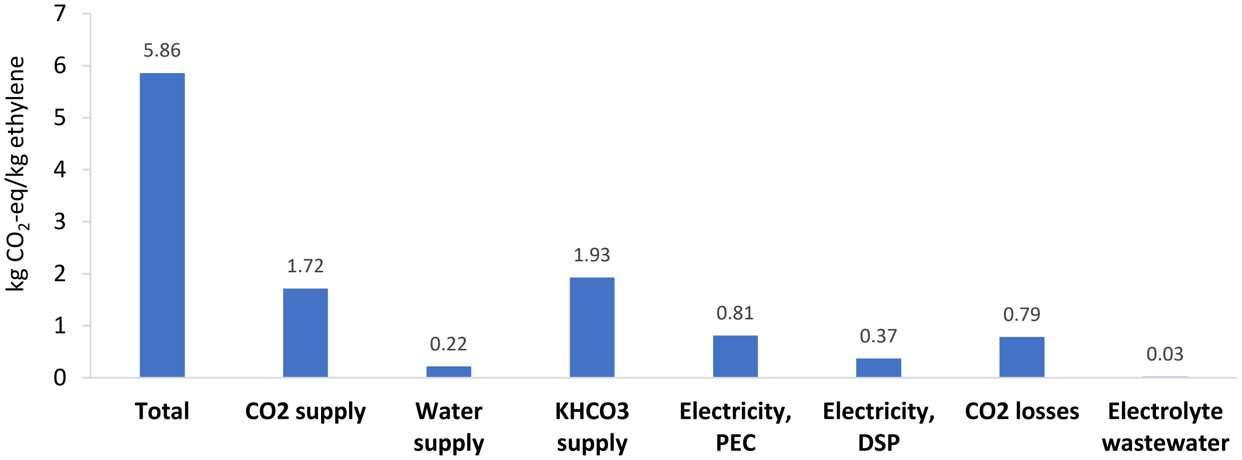

Figure 16. Contribution analysis for LICROX operation in the indicator of global warming.

In Figure 16 it can be seen that in terms of GHG emissions, plant operation has three main ‘hotspots’, namely potassium bicarbonate supply, CO_2 supply and electricity consumption. These three activities are responsible of 82% of the total GHG emissions associated to plant operation.

As in the indicator of respiratory inorganics, supply of potassium bicarbonate used in the PEC electrolyte is the single most important contributor to global warming. The preparation of the electrolyte is also the main water-consuming activity. If the two contributions are added ($KHCO_3$ supply plus water supply), it turns out that electrolyte preparation is responsible for 37% of the plant operation’s impact on global warming. As it has already been mentioned in section 4.3.2, the volume of electrolyte is expected to be replaced on a weekly basis, resulting in a specific consumption of 0.95 kg potassium bicarbonate per kg ethylene produced, together with 94.5 L ultrapure water.

Even though CO_2 is an industrial by-product, its recovery from flue gases, pressurization and transport still involves an expenditure in chemicals (monoethanolamine), energy carriers and pipeline infrastructure which, according to our model, results in a CO_2-eq footprint of 0.44 kg CO_2-eq/kg CO_2 supplied. Under the assumption of 80% efficiency in the utilization of CO_2 by the LICROX plant, this results in a CO_2-eq footprint of 1.72 kg CO_2-eq/kg ethylene.

Electricity supply is also a substantial contributor to GHG emissions. It has been estimated that the plant consumes 5.4 kWh/kg ethylene, with 69% of this associated to PEC operation and 31% to the DSP unit. These activities combined represent 20% of the net GHG emissions associated to plant operation as a life cycle stage.

4.5 Sensitivity analyses

4.5.1 Sensitivity to PEC photoanode material choice

The LICROX consortium is interested in finding out about the environmental consequences of the choice of photoanode materials used in the PEC. As a default, in this study it has been considered that the photoanode is based on $BiVO_4$, although the consortium has provided primary data to consider an alternative material, namely pseudobrookite nanoparticles (see section 3.1.12). In the inventory analysis, data for manufacturing a PEC incorporating these nanoparticles has been reported in several tables in section 3.1. In this sensitivity analysis, the life cycle impact of this alternative choice is assessed. The overall inventory for producing 1 kg ethylene by the LICROX technology remains the same as in Table 36, with the exception that the data set 'PEC, $BiVO_4$ {EU}' is replaced by the data set 'PEC, TiFe2O5 {EU}' (see Table 6). All figures in Table 36 remain the same. It must be highlighted that this analysis does not take into account any potential differences in performance by the PEC as a result of this shift. No such differences have been reported by the consortium.

Table 42.Impact assessment results at mid-point level for the default scenario (LICROX – $BiVO_4$) and for a scenario where the PEC uses $TiFe_2O_5$ in the photoanode (LICROX – $TiFe_2O_5$)

Indicator	Unit	LICROX – $BiVO_4$	LICROX – TiFe2O5
Human toxicity, carcinogens	kg C_2H_3Cl-eq	0.222	0.222
Human toxicity, non-carcinogens	kg C_2H_3Cl-eq	0.396	0.395
Respiratory inorganics	kg $PM_{2.5}$-eq	0.015	0.015
Ionizing radiation	Bq C-14 into air	121	121
Ozone layer depletion	kg CFC11-eq	5.09E-07	5.10E-07
Ecotoxicity, aquatic	kg TEG-eq into water	2383	2390
Ecotoxicity, terrestrial	kg TEG-eq into soil	96	96
Nature occupation	PDF·m^2·yr	0.001	0.001
Global warming	kg CO_2-eq	5.39	5.38
Acidification	m^2 UES	0.68	0.68
Eutrophication, aquatic	kg NO_3-eq	0.09	0.09
Eutrophication, terrestrial	m^2 UES	0.96	0.96
Respiratory organics	Person·ppm·h	0.0058	0.0054
Photochemical ozone, vegetation	m^2·ppm·h	61	57
Non-renewable energy demand	MJ primary	146	146
Mineral extraction	MJ extra	0.91	0.91

Table 42 shows the results of this analysis, where it can be seen that the results with the alternative photoanode material $TiFe_2O_5$ do not lead to a substantial change in the net impact per kg ethylene produced. In 13 out of the 16 assessed indicators, the impact score remains the same than when the $BiVO_4$ photoanode is used. The largest observed change is in the indicator of respiratory organics, where a reduction of 7% in the impact score is registered. It can be concluded that, with the available information for this study, the choice of $BiVO_4$ or $TiFe_2O_5$ as photoanode material is expected to have a minor effect in the life cycle impacts of the LICROX technology. The main reason for this is that these materials, even if having a relatively high footprint (as an example, 1 kg pseudobrookite nanoparticle dispersion in isopropanol leads to 172 kg CO_2-eq), are used in very small quantities in the PEC, which in turn is expected as a default to last 10 years. Thus, the impact of such materials per kg ethylene becomes very low when compared to other activities in the life cycle. As already mentioned, this analysis considers that the two photoanode options lead to the same technical performance. If in reality it can be eventually proven that one option has a superior performance, leading to e.g. a higher ethylene yield or a higher stability of the device, it would be justified to choose it as this higher performance would likely be translated into a better environmental performance too.

4.5.2 Sensitivity to impact assessment method

In this section we assess the two alternative ethylene production systems using an alternative impact assessment method at the mid-point level, namely the one proposed by the European Commission, Joint Research Centre, in the framework of the International Reference Life Cycle Data System (ILCD) (Hauschild et al. 2011). This method was implemented by Pré Sustainability in the SimaPro software, where it is labelled 'ILCD 2011 Midpoint+'. This method includes a total of 16 environmental impact indicators.

Table 43.Impact assessment results at mid-point level with the ILCD 2011 Midpoint+ method

Indicator	Unit	Steam cracking	LICROX
Climate change	kg CO_2 eq	0.25	5.31
Ozone depletion	kg CFC-11 eq	1.0E-06	5.1E-07
Human toxicity, non-cancer effects	CTUh[a]	6.2E-07	5.2E-06
Human toxicity, cancer effects	CTUh[a]	8.2E-08	1.4E-06
Particulate matter	kg $PM_{2.5}$ eq	0.0016	0.0069
Ionizing radiation, human health	kBq U235 eq[b]	0.83	1.19
Ionizing radiation, ecosystems	CTUe[c]	4.3E-06	3.1E-06
Photochemical ozone formation	kg NMVOC eq[d]	0.0041	0.0282
Acidification	mol H^+ eq[e]	0.010	0.051
Terrestrial eutrophication	mol N eq[f]	0.016	0.113
Freshwater eutrophication	kg P eq[g]	0.0009	0.0101
Marine eutrophication	kg N eq[f]	0.0015	0.0122
Freshwater ecotoxicity	CTUe[e]	56	589
Land use	kg carbon deficit	19	31
Water resource depletion	m^3 water eq	0.0577	-0.0076
Mineral, fossil and renewable resource depletion	kg Sb eq[h]	0.000035	0.003206

[a] CTUh: comparative toxic unit, humans; [b] KBq U235: kilobecquerel Uranium 235; [c] CTUe: comparative toxic unit, ecosystems; [d] NMVOC: non-methane volatile organic carbon; [e] H^+: hydrogen ion; [f] N: nitrogen; [g] P: phosphorus; [h] Sb: antimony.

Table 43 above displays the results of this sensitivity analysis, where the results per kg ethylene are shown for each of the 16 indicators in the ILCD 2011 method. The absolute figures shown for both LICROX and petrochemical ethylene are not expected to match those in Stepwise, given that the underlying characterization models and the units used are in many cases different. The analysis is useful, however, in order to find out whether or not the same ranking pattern is observed as when Stepwise is used. The answer to this question is affirmative, in the sense that in a majority of indicators (14 out of 16) the LICROX technology appears to have a higher impact than steam cracking. On the other hand, favourable results for LICROX appear in the following indicators:

- Ozone depletion: this is consistent with the results obtained for the same indicator in the Stepwise method.
- Ionizing radiation, ecosystem effects: this particular indicator is not addressed by the Stepwise method, which addresses ionizing radiation from the perspective of human health effects only. It can be seen that the ILCD 2011 results for ionizing radiation effects on human health are aligned with those of the equivalent indicator in the Stepwise method (Ionizing radiation).

- Water resources depletion: this particular indicator or an equivalent one is not included in the Stepwise method, which does not currently address water resources. The lower impact of LICROX seems to be related to avoided water use as a result of recycling steel present in the LICROX plant infrastructure. A closer inspection of these results reveals that they do not appear as a consequence of LICROX using less water in its life cycle (in fact, at the inventory level the net use of water by LICROX is higher than for steam cracking), but as a result of the water scarcity factors applied to water flows in different regions of the World, which the ILCD 2011 method took from the Swiss Eco-scarcity method 2006 (Frischknecht et al. 2009). It must be highlighted that the Swiss Eco-scarcity method 2006 can be considered outdated and therefore these results are not considered robust enough to conclude on a potentially lower water footprint of LICROX when compared to steam cracking.

If we take a closer look at the indicators that have been identified by Stepwise as most relevant when applying weighting by monetarization (global warming and respiratory inorganics), these would correspond in the ILCD 2011 method to 'Climate change' and 'Particulate matter'. In Climate change, the CO_2-eq figures obtained with the ILCD 2011+ method are different to those in Stepwise, since the former relies on the global warming potentials published by the Intergovernmental Panel on Climate Change (IPCC) in 2007, while Stepwise uses those published in 2013. Regarding particulate matter, the absolute $PM_{2.5}$-eq figures are lower than in Stepwise, but with both methods LICROX appears to have approximately 4 times higher score than steam cracking.

4.6 Environmental improvement analysis

The life cycle impact assessment results show that the LICROX concept for production of ethylene, as proposed in this study, involves a substantially higher environmental impact than production of ethylene by steam cracking. However, as mentioned in the goal of this study, one of such goals is to provide suggestions to steer this technology towards a lower environmental impact. In this section we consider a set of changes in the life cycle model, aimed at reflecting a reduction in environmental impacts. The options considered are based either on consortium suggestions, such as the direct supply of carbon dioxide from flue gas, as well as on insights from the life cycle impact assessment results, where clear hotspots have been identified. In the following sections the individual changes are described together with inventory data implications. The results of this analysis are given in section 4.6.5. To simplify the interpretation of results, we focus on the global warming indicator only.

4.6.1 Electrolyte replacement

The electrolyte replacement frequency is subject to substantial uncertainty. In the first iteration of this LCA study, a daily replacement was suggested by the LICROX consortium, leading to this particular aspect dominating the life cycle impacts in the preliminary results of the study. For this second iteration, given the potential importance of this aspect, the consortium has suggested instead a weekly replacement frequency, and pointed to the fact that a daily replacement was taken only as a worst case. In this improvement analysis it is assumed that the electrolyte has a longer durability, allowing for an annual replacement being sufficient. According to the consortium, such lower frequency cannot be ruled out at this point, but it cannot be guaranteed either. This analysis anyway aims at understanding how much this improvement means on a life cycle basis. This alternative scenario involves the following changes in the plant operation inventory:

- Consumption of potassium bicarbonate and ultrapure water, quantified at 0.95 kg and 94.5 L per kg ethylene in section 3.3.3, are reduced to 0.02 kg and 1.82 L, respectively.
- Production of electrolyte wastewater for disposal, quantified at 95.5 kg per kg ethylene, is reduced to 1.84 kg.

All other aspects of the life cycle inventory remain unchanged.

4.6.2 Ethylene yield

The ethylene yield as such has not been identified as a hotspot in the life cycle impact assessment results, however this single parameter implicitly affects most if not all inventory flows, since the yield is inversely proportional to the amounts of all materials, services, etc. required per unit of ethylene product. In this analysis the yield is arbitrarily doubled, from 0.015 to 0.030 kg ethylene/m^2 PEC/day, keeping everything else constant, just as an example to evaluate the influence of this parameters in the results.

From an inventory analysis point of view, changing the yield affects the following activities in the model:

- PEC production and PEC disposal, quantified at 0.0203 m^2 PEC per kg ethylene in section 3.5, are reduced to 0.01015 m^2 PEC per kg ethylene.
- PEC infrastructure and PEC infrastructure disposal, quantified at 0.203 m^2 PEC-year per kg ethylene in section 3.5, are reduced to 0.1015 m^2 PEC-year per kg ethylene.
- Consumption of potassium bicarbonate and ultrapure water, quantified at 0.95 kg and 94.5 L per kg ethylene in section 3.3.3, are reduced to 0.47 kg and 47.3 L, respectively.
- The resulting volume of electrolyte wastewater is also reduced, from 95.5 kg per kg ethylene to 47.8 kg per kg ethylene.
- Electricity consumption for PEC operation, quantified at 3.67 kWh per kg ethylene in section 3.3.3 , is reduced to 1.83 kWh per kg ethylene.
- Tap water for PEC cleaning, quantified at 5.07 L/kg ethylene in section 3.3.5, is reduced to 2.54 L per kg ethylene.

All other aspects of the life cycle inventory remain unchanged.

4.6.3 Photovoltaic energy

With LICROX constituting a solar-assisted photochemical process, a potential option to consider in a hypothetical production plant design is to make it fully solar, by also powering all the plant equipment with photovoltaic energy produced onsite, instead of with grid electricity.

In this analysis, the total electricity consumption for plant operation, quantified at 5.4 kWh per kg ethylene, is linked to the ecoinvent data set for a photovoltaic plant installed on open ground with a 570 kWp capacity. The ecoinvent database provides inventories, on a per kWh basis, for 10 European countries[1]. In this analysis we consider the productivity of this hypothetical plant as the arithmetic average for these 10

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[1] Austria, Belgium, Germany, Spain, France, UK, Italy, Netherlands, Portugal and Sweden.

countries. The calculated consumption of photovoltaic plant infrastructure is 6.23E-08 plant units per kWh supplied during its lifetime.

In addition, given that photovoltaic installations are land-demanding, in the inventory we also include their potential iLUC effects, assuming each m^2 of photovoltaic panel installed involves a land occupation of 4.7 m^2-year, as considered in the ecoinvent database for open-ground installations. This land occupation can then be linked to the iLUC inventory in section 3.2.3. The calculated iLUC flow for this hypothetical average photovoltaic installation is 7.39E-04 kg NPP_0 as carbon/kWh supplied.

4.6.4 Carbon dioxide from flue gases

By request from the LICROX consortium, a scenario is considered where carbon dioxide is supplied to the production plant in the form of unprocessed flue gases from a natural gas-fired power plant. The technical feasibility of such a scenario is far from proven, given that flue gases contain minor concentrations of pollutants that might interfere with the catalysts in the PEC device, leading to unwanted side effects such as a decrease in process efficiency or in the useful life of the materials. Such side effects are not included in this analysis, nor are any implications in re-dimensioning the PEC to handle the higher flow of gases it would need to receive.

From an inventory analysis point of view, supply of carbon dioxide, quantified at 3.93 kg/kg ethylene in section 3.3.1, is included in the model with the data in Table 28 for carbon dioxide in flue gas, instead of pressurized carbon dioxide. In addition, an attempt has been made to include in this analysis the implications of such a change in the downstream processing unit. Given that carbon dioxide only represents 14% of the mass of flue gas, the DSP unit now needs to process a much higher volume of gases from the PEC. A re-working of the plant's mass and energy balance has been performed, in order to quantify this change, as shown in Figure 17.

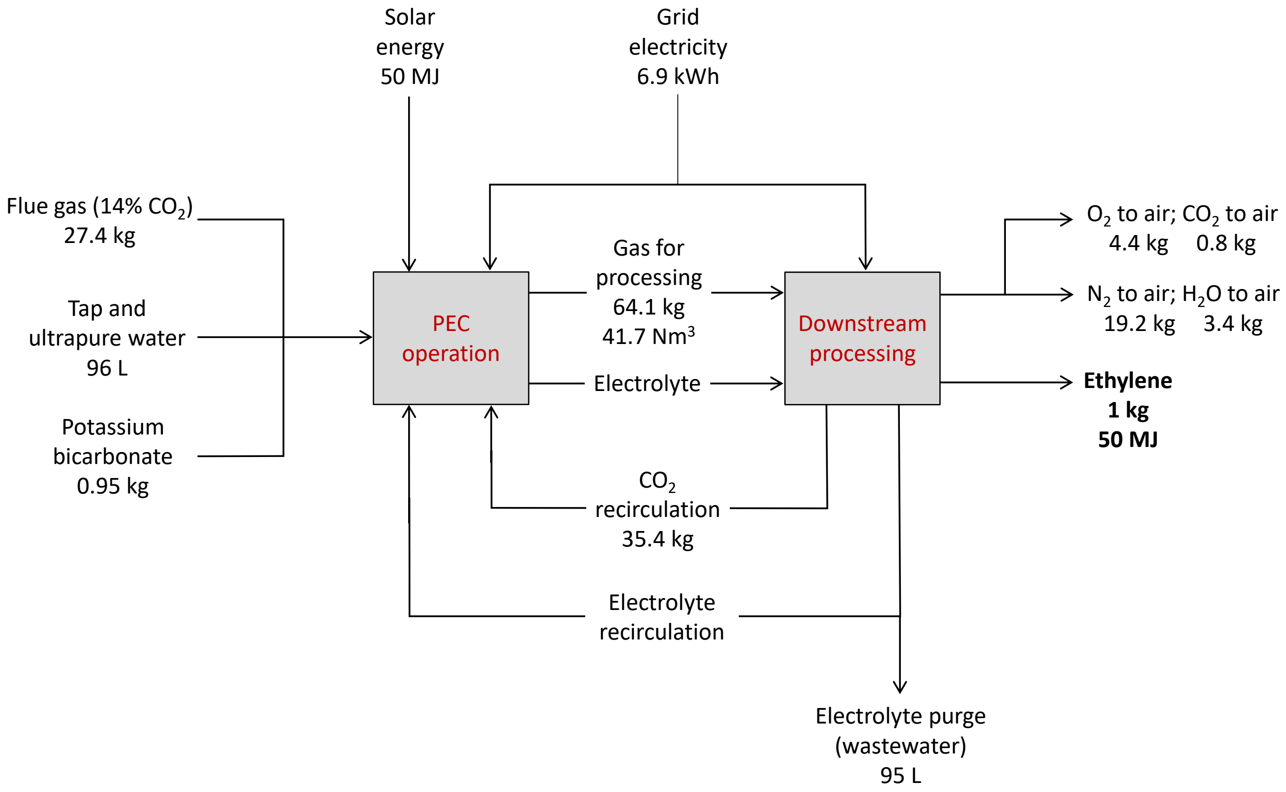

Figure 17. Mass and energy balance for the LICROX plant operation in a scenario where unprocessed flue gas from a natural gas-fired power plant is used as carbon dioxide source.

In Figure 17 it can be seen that the volume of gas to be processed when flue gas is used is 41.7 Nm^3 per kg ethylene, compared to 21.5 Nm^3 when pure carbon dioxide is used (Figure 8). In the life cycle model, this affects the following activities in the inventory:

- DSP infrastructure and DSP infrastructure disposal, quantified at 21.5 Nm^3 per kg ethylene in section 3.5, increase to 41.7 Nm^3 per kg ethylene.
- Electricity consumption for DSP operation is assumed to increase linearly as a result of the higher volume of gas to be processed. Thus, this consumption increases from 1.67 kWh per kg ethylene, as quantified in section 3.3.8, to 3.24 kWh per kg ethylene. This means the total electricity consumption of the LICROX plant increases to 6.9 kWh, as shown in Figure 17.

All other aspects of the life cycle inventory remain unchanged.

4.6.5 Results of the environmental improvement analysis

The results of the improvement analysis are shown in Figure 18, for the indicator of global warming. In this figure, the default results for steam cracking and LICROX are shown, followed by the results for LICROX after considering the individual improvements described in sections 4.6.1 to 4.6.4. The last result in Figure 18 represents the combination of all individual improvements together.

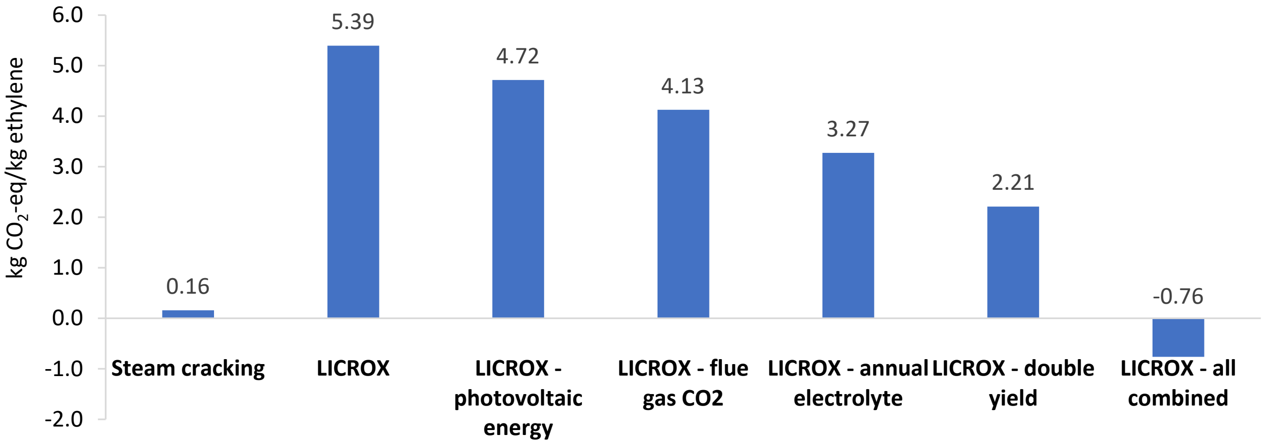

Figure 18. Results for the improvement analysis in the indicator of global warming.

In Figure 18, improvements to LICROX have been ranked from left to right, according to the magnitude of GHG emission reduction. The results for each individual improvement can be summarized as follows:

- The implementation of photovoltaic energy reduces GHG emissions by 0.68 kg CO_2-eq/kg ethylene (13% reduction). It must be borne in mind that electricity supply has not been identified as the biggest hotspot in the life cycle, and therefore a change to this aspect is not expected to lead to a major change. Another aspect to bear in mind is that, even though photovoltaic electricity involves lower GHG emissions per KWh supplied (0.094 kg CO_2-eq/kWh in our model for Europe) than grid electricity, the difference with the grid electricity mix in Europe in the ecoinvent database is not so big (at 0.222 kg CO_2-eq/kWh). This is due to the fact this electricity mix does not consider the average supply to the grid, but the marginal supply instead, which is expected to already account for a substantial share of renewable electricity sources.
- The substitution of pure carbon dioxide by dilute CO_2 in flue gases reduces GHG emissions by 1.27 kg CO_2-eq/kg ethylene (24% reduction). This reflects the savings in energy consumption by avoiding carbon dioxide capture and pressurization, even though it also leads to higher impact in the DSP unit, due to the higher volume of gases to be processed. Again, it must be borne in mind that this shift in carbon dioxide source has been assumed not to affect in any way the design or operation of the PEC, which might be optimistic.
- The reduction in electrolyte replacement, from weekly to annually, leads to a reduction of GHG emissions by 2.12 kg CO_2-eq/kg ethylene (39% reduction). This aspect has been identified as clear hotspot in the life cycle, and therefore the suggested change leads to substantial reduction in GHG emissions, given that activities related to electrolyte production and disposal as wastewater are reduced by a factor 52.
- The doubling of the ethylene yield appears to be the individual change, from the ones proposed, leading to the highest reduction in GHG emissions, namely 3.18 kg CO_2-eq/kg ethylene (59% reduction). It can be easily seen that doubling the process productivity, without increasing the amounts of inputs, leads to a halving of the environmental footprint per unit of product. Thus, it is clear that improving the ethylene yield should be one of the priorities by the LICROX consortium.

- The last column in Figure 18 shows the hypothetical GHG emissions of a LICROX plant where all the above-discussed improvements are combined. It can be seen that in such a scenario, the footprint of LICROX becomes negative, meaning a net GHG emission saving, of 0.76 kg CO_2-eq/kg ethylene. Here it is worth mentioning that LICROX appearing as a net CO_2 sink is just a result of the cradle-to-gate boundaries of the study. In a cradle-to-grave study, LICROX could register CO_2 emissions from the degradation or combustion of ethylene (for example, if incinerated), leading to a net life-cycle GHG emission of positive rather than negative sign. What stays the same, regardless of the study boundaries, is the difference between steam cracking and LICROX: in this optimistic scenario, replacing 1 kg petrochemical ethylene by LICROX ethylene saves a total of 0.16 + 0.76 = 0.92 kg CO_2-eq.

4.7 Sensitivity, completeness and consistency checks

According to ISO 14044 an evaluation in the interpretation phase including sensitivity, completeness and consistency check must be carried out in order to establish confidence in the results of the LCA study.

4.7.1 Completeness check

A completeness check is presented to ensure that the full required information and data from all phases have been used and are available for interpretation, including the identification of data gaps.

The study excludes the use and disposal of ethylene in finished products. This is justified on the basis that these life cycle stages are not affected by the choice of ethylene production technology. The only difference associated to the end-of-life stage is that carbon in ethylene from steam cracking is of fossil origin, while carbon in LICROX ethylene can be considered in the same way as ‘biogenic’ carbon, i.e. carbon taken from the atmosphere that is ultimately re-released with a net zero effect on global warming. This can be considered for LICROX as it uses CO_2 that would have been otherwise emitted to the atmosphere, equally resulting in a net zero effect on global warming. This aspect would be typically included at the end-of-life stage, when the ultimate fate of carbon (landfilled, incinerated, etc.) is assessed. Since this life cycle stage is excluded in this study, this aspect is included as a CO_2 credit to LICROX, calculated based on the amount of carbon in ethylene, leading to an avoided emission of -3.14 kg CO_2/kg ethylene. This can be seen as a form of system expansion.

Regarding foreground data for steam cracking, the data have been obtained from published literature (Rodríguez-Vallejo et al. 2020), providing a sufficiently detailed mass and energy balance for steam cracking and for propylene production using methanol as feedstock. The mass and energy balances provided by Rodríguez-Vallejo et al. (2020) originated from process simulation using the Aspen HYSYS software. Some aspects not originally included by these authors have been included in the present study, such as infrastructure, iLUC effects and steam cracker direct emissions to air other than carbon dioxide.

Regarding LICROX, the foreground data available directly from the consortium were incomplete, given that this technology is still under development, and not even a prototype has been built yet. Foreground data by the consortium mainly referred to material composition and manufacturing processes for the PEC, based on lab-scale data, expected manufacturing processes and literature. Data on other infrastructure needed to build a LICROX plant were non-existent, and this gap was filled by using data from a similar technology applied at industrial scale, namely a solar-assisted photocatalysis plant installed in Spain. Data on LICROX plant operation were equally scarce. A mass balance has been established based on the process stoichiometry and expected operation procedures foreseen by the consortium, such as the use of industrial CO_2, its utilization efficiency or the need to replace electrolyte on a weekly basis. Energy use by this plant was available from the consortium as plausible values. A similar gap occurs for downstream processing of the produced gases, processed in a pressure swing adsorption unit. Literature data for an industrial plant treating biogas have been used to characterize such infrastructure. iLUC effects have been included, based on the estimated land occupation by the plant. Overall, the developed model can be said to cover all the required aspects: PEC and plant infrastructure, operation and dismantling, however the reliability of this model to represent an actual deployment of this technology at a commercial scale is questionable. Yet, the available information can be used to get a first glimpse of the environmental profile of this technology, and of how to improve it.

Regarding background data, the life cycle inventory is based on the ecoinvent database. This database presents certain limitations regarding completeness: capital equipment is included to a limited extent, while services (economic activities such as banking, legal advice, retail, education, etc.) are not included. Ecoinvent, as a traditional LCA database, focuses instead on material and energy flows of industrial activities. A more complete inclusion of capital and services in the background could be achieved by using an input-output LCA database, but this option was ruled out as these databases are by default too aggregated in order to be used in a study like this one, requiring the assessment of many uncommon materials.

At the impact assessment level, the Stepwise method has been used, which addresses a wide variety of environmental issues. On top of this, an additional assessment with the ILCD 2011+ method has been performed. Both methods point to similar conclusions at the mid-point level.

Potential environmental rebound effects associated to differences in life cycle cost have not been included, given that assessing life cycle costs was not in the scope of this study.

4.7.2 Consistency check

The objective of the consistency check is to verify that assumptions, methods, and data are consistent with the goal and scope of the LCA study. Especially, the consistency regarding data quality along the product chain, regional and temporal differences, allocation rules/system boundaries and impact assessment are important, according to ISO 14044.

In general, the life-cycle inventory model is based on a consistent and well-defined methodological framework as presented in section 2, namely for consequential LCA. In the foreground, constrained activities are excluded, and multifunctionality is handled by substitution. This applies to both steam cracking and LICROX. In the background, the same choices are applied by the consequential system model of the ecoinvent database.

Inclusion of iLUC is not consistently applied throughout the product system, but only in the foreground. A consistent implementation would only be possible by having the iLUC model of Schmidt et al. (2015)

applied in the entire ecoinvent database. In this study, the main iLUC effects were expected for the LICROX technology, as the plant is potentially land-demanding. The results, however, seem to suggest that iLUC is much less of a hotspot than other aspects.

4.7.3 Sensitivity check

In section 4.5, two sensitivity analyses have been performed, namely on the choice of photoanode materials used in the PEC, and regarding the impact assessment method used in the study. The LICROX technology shows very little sensitivity to changes in the choice of photoanode materials. The overall impact per kg ethylene produced remains largely unchanged when $TiFe_2O_5$ is used instead of $BiVO_4$. In most impact indicators, changes in impact assessment results are below 1%. Regarding sensitivity to impact assessment method, the results at mid-point level when using the Stepwise and the ILCD 2011 methods are in agreement when it comes to the relative ranking of LICROX vs. steam cracking.

In addition, the improvement analysis performed in section 4.6 can also be understood as a sort of sensitivity analysis, focused on those aspects that are expected to dominate the life-cycle impacts of LICROX. A total of four individual parameters have been tested, showing that the ethylene yield (in kg/m^2 PEC/day) is likely to be the most sensitive parameter for this technology, followed by the frequency of electrolyte replacement.

The results of the study are also expected to be sensitive to the choice of life cycle inventory modelling approach (consequential vs. attributional). In steam cracking, for example, an attributional approach using mass allocation, as done by PlasticsEurope (2012) and the US LCI database (NREL 2022) shows a global warming impact for ethylene of approximately 1.2 kg CO_2-eq/kg ethylene, while in this study the value obtained, using a consequential approach, is 0.16 kg CO_2-eq/kg ethylene, that is 7.5 times lower. For ethylene produced by LICROX, the system is not expected to show such a high level of sensitivity to the modelling choices, as there are no co-production issues, but absolute scores in most, if not all, indicators would be expected to be higher in an attributional framework, given that, for example, credits associated to substitution are not considered, and electricity production mixes are expected to include a higher share of fossil-based power production, which are often considered constrained in a consequential perspective.

4.8 Conclusions, limitations and recommendations

The main conclusions of the present study can be summarized as follows:

- Life cycle impacts from ethylene produced by a hypothetical LICROX production plant, as envisaged in this study, appear to be substantially higher than those for ethylene produced by conventional steam cracking. This is the case for 15 out of the 16 indicators included in Stepwise. As an example, GHG emissions are 34 times higher for LICROX.

- The main driver for environmental impacts of the LICROX technology corresponds to plant operation. Two main aspects are highlighted as key contributors: electrolyte supply and CO_2 supply. The impact of electrolyte supply is closely related to the fact that potassium bicarbonate and ultrapure water need to be added and replaced on a weekly basis, while the impact of Carbon dioxide supply mainly corresponds to the energy use associated to recovering this gas from industrial exhaust gases.

- The environmental impact associated to the PEC as a component of the LICROX plant is not negligible. It can be considered as the second most important aspect after plant operation, and this is closely related to the relatively low ethylene yield. The environmental impact of the PEC is highly dependent on the assumed useful life, which has been taken as 10 years. However, this degree of durability is currently more a hope or a goal than a fact. The main identified contributor to the environmental impact of PEC as a component is the electricity consumed during its manufacturing.

- Other plant infrastructure construction and disposal (including the downstream processing unit) appear to also be relevant, but this is partly offset by the fact that many materials in this infrastructure are expected to be recycled when the plant is dismantled. This mitigates the life-cycle impact. The environmental relevance of infrastructure is closely linked to the relatively low ethylene yield by the plant.

- The role of energy consumption in the life-cycle impact is also relevant, quantified at 5.4 kWh/kg ethylene, assumed to be supplied by the grid. This aspect appears is ranked third in terms of GHG emissions related to plant operation, after electrolyte supply and carbon dioxide supply.

- The choice of photoanode material to be used in the PEC, namely $BiVO_4$ of $TiFe_2O_5$, seems to have very low influence on the overall life cycle impact of ethylene production by LICROX. This is mainly due to the fact that these materials are used in very low quantities.

The main limitations of this study can be summarised as follows:

- At this stage, the LICROX consortium knows too little about what a commercial LICROX production plant will look like, which has led in this study to a general lack of primary data on many aspects, such as production of many underlying materials used in the PEC, infrastructure of a LICROX plant, energy consumption by such a plant, etc. This has been overcome with expert judgement by the consortium and 2.-0 LCA consultants, filling all gaps with the most appropriate available information. In spite of this, the uncertainty in the results is high: aspects that are judged in the results as having low priority could be in reality more important, and vice versa.

The main recommendations to the LICROX consortium are the following:

- In order for the LICROX technology to reduce its life-cycle impact, the most important identified parameter to improve is the ethylene yield by the PEC (in kg /m^2 PEC/day). Doubling this yield effectively halves the impact of many activities on a per kg ethylene basis. Other measures aimed at reducing this impact, in order of importance, are: reducing the electrolyte replacement frequency, using unprocessed flue gases as source of carbon dioxide, and the use of photovoltaic electricity to operate the plant. Nevertheless, the technical feasibility of implementing such improvements needs to be ultimately confirmed by the LICROX consortium.

- To conduct a theoretical scale up of the LICROX prototype that includes all unit operations expected in an industrial production plant, to validate this study. Such a scale up could be used as the basis for a more reliable application of LCA.

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Appendix: critical review report

1st iteration: reviewer comments

Critical review report of the study:
“Life cycle assessment of the LICROX technology”
By Miguel Brandão, PhD
16th April 2022

1. Introduction

The present document reports the review made to a life cycle assessment (LCA) study of the LICROX technology. The LCA study in question (Muñoz, 2022) was performed by Ivan Muñoz, from 2.-0 LCA consultants, and commissioned by the EU-funded HORIZON2020 project consortium, under which the LICROX technology is being developed. This is the revision of the first iteration, sent on 1st April, and sent back on 16th April.

LICROX is a scientific project in which photoelectrochemical cells are being developed to mimic natural photosynthesis and allow for a sustainable formation of ethylene. As part of this project, an LCA of the LICROX technology will be conducted to estimate its impacts on 16 environmental categories (following the stepwise method).

The LCA study reviewed consists of the first iteration related to the definition of scope and life cycle inventory. Furthermore, results are estimated for the distribution of 1 kg of ethylene, and compared with a more traditional way of producing ethylene (i.e. steam cracking).

2. Scope of the review

This review characterises the study against a fixed set of criteria that are commonly used in LCA reviews and can be found in the ISO standard 14071 (ISO, 2014). These characteristics cover each of the four phases of LCA, and this review is structured around those: 1) goal & scope definition, 2) inventory analysis, 3) impact assessment and 4) interpretation. This review covers the first two phases of the LCA.

This critical review ensures that the methods used to carry out the LCA are consistent with the ISO standards - 14040 (ISO, 2006a), 14044 (ISO, 2006), as well as technical specification (TS) 14071 (ISO, 2014) – and are scientifically and technically valid. It also ensures that the data used are appropriate and consistent with the goal and scope of the study. Finally, this review ensures the first iteration of the LCA report is transparent and consistent. All these features are required by TS14071 (ISO, 2014) and represent the checks and balances that ensure the quality of the study.

This review is performed based on expert review. It has been performed at the middle of the study, but changes are expected to occur after the production of this report, which will be reassessed as follows (5-stage procedure) for each iteration:

1. Reviewer reads and comments on the report
2. Study authors will go through reviewer comments one by one and make a revised report and an itemized reply
3. Reviewer reads the authors’ itemized reply and give any potential remaining comments
4. Authors will go through any remaining issues the reviewer might have and make a revised LCA report and itemized reply

5. Reviewer reads author’s revised itemized reply and makes final review statement (applicable only to the final iteration).

This review report corresponds to step 1 above and pertains the first iteration, which was sent on 1st April 2022. It excludes a detailed assessment of the life cycle inventory (LCI) model and of the individual data sets but, as required by TS14071 (ISO, 2014), it covers all aspects of the LCA’s definition of scope and life cycle inventory (LCI), including data appropriateness and reasonability, calculation procedures and calculated LCI results.

It is outside the scope of this review to address the goals chosen for the LCA study in question, as it is impossible to either verify or validate them. The responsibility for those, as well as the ways in which the LCA results are used, lie with the commissioner of the LCA study. Specific comments to the definition of scope and life cycle inventory study are be provided in Table 1.

3. Review of LCA study of the LICROX technology

Goal and scope definition

LCA practice is standardised by the International Organization for Standardisation (ISO) in ISO14040 (ISO, 2006a) and ISO14040 (ISO, 2006b). These standards include the terminology and requirements for LCA studies, such as the process for conducting LCA studies, methods, data, evaluation, documentation, etc. ISO compliance ensures that the study adheres to those internationally-agreed rules and, thus, credibility and bias-freedom. However, it may not necessarily ensure scientifically soundness and robustness.

This section of the study covers an explanation of what this particular stage is and where it falls within the four phases of an LCA. It also includes a description of the process of the: critical review, purpose (including data collection, temporal and geographical scope), functional unit, life cycle inventory model and life cycle impact assessment (including the adopted environmental impact categories, as well as how biogenic emissions and indirect land use were dealt with), system boundaries and reference flows (which were clearly specified).

The following has been verified:

- The study under review claims to be compliant to the above standards. This is indeed attested.
- It is specified that the study will go through a critical review.
- The study’s goals are clearly formulated, as are the intended application and audience.
- Data collection follows concerns of consistency.
- The temporal scope is specified.
- The geographical scope is delimited to Europe for the foreground system, while inputs to the foreground come from the rest of the world in an average-global manner.
- The functional unit is specified and is appropriate. It will be used for comparison purposes.
- It is clearly stated the LCI model follows a consequential approach and an explanation
- of the approach is given.

- It is clearly stated that the LCIA method used is Stepwise 2006 and an explanation of the method and updated are given. A comprehensive set of environmental impact categories was adopted and identified.
- Treatment of biogenic carbon and methane is explained and justified properly.
- Nature occupation is modelled consistently with that of iLUC.
- System boundaries delimitation: cut-off as Input-Output databases are not used. The exclusion of the use-phase and of the end-of-life phase is justified and correct.

Life cycle inventory (LCI)

This section describes the data and modelling in the reviewed LCA study. It starts by making a distinction between the foreground and background systems. Subsequently, it explains the use of ecoinvent for the background data, and a general description of that database. The consequential system model version used ensures consistency with the consequential approach.

Indirect land use changes (iLUC) – which are often neglected in LCA – are modelled in a consistent way with the rest of the LCA model.

Other general activities related to production (photoanode, photocathode, OPV), infrastructure, inputs (electricity, chemicals and water), plant (operation and disposal) and wastewater treatment, are described appropriately. Care was taken to avoid inappropriate double-counting.

The involved activities are described and inventory summaries shown, including photoelectrochemical cell manufacturing, plant infrastructure, operation, disposal, as well as those related to the alternative way of producing ethylene: steam cracking.

Conclusions

The review of the goal and scope definition and LCI phases of the study on the LICROX technology revealed an extremely competent analysis that underwent the rigorous application of the aforementioned ISO standards. Thus, it can be inferred that the first part of the study reviewed is an ISO-compliant, consistent and scientific application of the LCA methodology.

Given the infant nature of this technology, and associated inexistent of specific data, the author went into great lengths to ensure the best possible representativeness of the data used. Robust-enough approximations were used throughout the study, which only attests to the high competence of the study.

I therefore conclude that the study made so far is of high quality, and once concluded can support environmental decision making.

References

Muñoz I (2022) Life Cycle Assessment of the LICROX technology. First iteration: Definition of scope and life cycle inventory. 2.-0 LCA consultants, Barcelona, Spain.

ISO 14040 (2006) Environmental management – Life cycle assessment – Principles and framework.

International Standard Organization (ISO), Geneve.

ISO 14044 (2006) Environmental management – Life cycle assessment – Requirements and guidelines. International Standard Organization (ISO), Geneve.

ISO 14071 (2014) Environmental management – Life cycle assessment – Critical review processes and reviewer competencies: Additional requirements and guidelines to ISO 14044:2006. International Standard Organization (ISO), Geneve.

Table 1: Detailed comments (ed: editorial; te: technical).

Index	Paragraph/ Figure/Table	Type of comment	Reviewer comment	Reviewer recommendation	Author of the LCA study response
Goal and scope definition					
#1	Section 1.1	ed	Wrong choice of word?	Replace "fabricate" with "produce". "Fabricate" is usually used in the context of producing misleading and inaccurate data.	
#2	Section 1.2	te	The scope may have been exaggerated.	Can the study really say whether the LICROX technology is sustainable or not? Will a cost assessment be carried out?	
#3	Section 2.4	te	CO2 as a by-product	Is CO2 clearly a by-product? I think this is always the case but a justification may be warranted and, if not, results could be tested for their sensitivity to considering CO2 differently.	
#4	Section 2.5	te	Substitution	This is indeed the correct approach for a consequential LCA. A clear list of all marginal products that are assumed to be displaced (as well as their inventory) would be welcomed.	
#5	Section 2.7.1	te	Figure 3 excludes by-products (and substituted product systems).	Include main by-products and product systems displaced by these.	
#6	Section 2.7.2	te	Given that Europe is the focus geographical unit, why use global averages here?	Consider whether or not it makes sense to use a European-based average for the parameters currently using a World average ("average global scenario") for the supply of underlying materials.	
#7	Section 2.7.3	te	Reference system: consistency with the system boundary of LACROX	Ensure that the delimitation of the system boundary in both system (LICROX and that representing ethylene produced from steam cracking) is consistent.	
#8	Section 2.8.1	te	Issues of scale	Given that a not even a LACROX prototype exist, scaling is indeed challenging (as identified). Could a certain % increase in efficiency be assumed to reflect an established level of production?	
#9	Section 2.8.1 but subsequent sections as well	te	Efficiency assumptions	It may be optimistic to assume 100% efficiency in e.g. the use of CO2 and water.	
#10	Section 2.8.1	te	Assumption of CO2 input	How would the assumption of atmospheric CO2 affect the results (if at all)?	
#11	Section 2.8.1	te	Plant dismantling operation excluded	I trust the reference steam cracking plant dismantling operation is also excluded?	
#12	Section 2.8.2	te	Ecoinvent version 3 system model	Perhaps mention here that the ecoinvent system model of Ecoinvent is used?	
#13	Section 2.8.2	te	Consistency in how the two systems under comparison are modelled	I understand that the data from Franklin associates is used for the steam cracking model. But this system is delimited with reference to mass allocation, which may render it incomparable with the LACROX system under assessment.	
#14	Section 2.9	te	Consistency in the state-of-the-art of different impact categories	Stepwise 2006 is used with updates on some categories. Given that the method was developed 15 years ago, can you justify the choice of adopting it, especially in light of having only some, not all, impact categories updated, which may bring an issue of inconsistency. Furthermore, can you include a justification of why the hierarchist approach in ReCiPe 2013 was adopted?	
#15	Section 2.10.1	te	CO2 source and C sink Missing environmental mechanism?	See above. Is the timing of sequestration and emissions of GHGs accounted for in the sense that earlier flows have a larger GWP? I do not think that it is, but the iLUC model implicitly does this, so there may be an issue of consistency. The consideration of the CO2 input could be excluded if no differentiation vis-à-vis timing of emissions is made. If it is made, several methods exist that account for this. How is temporary carbon storage in landfills dealt with, if at all? Also, make sure that having a cradle-to-gate approach does not make the comparison erroneous and mass imbalanced.	
#16	Section 2.10.2	ed	iLUC	Define the term here?	
#17	Section 2.10.2	te	iLUC	iLUC does not assume only deforestation, as e.g. grassland is also part of the land supply mix. Referring only to deforestation may be misleading.	
#18	Section 2.10.2	ed	iLUC	NPP0 refers to potential NPP	

#19	Section 3.1	te	"unspecified European country"	What does this mean? Is it representative of the European (weighted) average?	
#20	Section 3.1.2 but applies to other sections too	te	Missing data	I understand that data may not exist to characterize such a novel technology. Some of these data are expected to be made available for the second iteration, but the level of "guesstimating" in this study is extremely high.	
#21	Section 3.1.4	te	Double counting	See comments above. It is important to make sure that CO2 accounting is consistent with the goal and scope and with the systems' delimitations.	
#22	Section 3.1.6, 3.1.7 and beyond	te	Missing data	See comments above. I understand data may not exist for all activities. Several approximations had to be incurred in throughout the study. In this section, is lead a good approximation for bismuth? Are data for vanadyl sulfate acceptably similar to that of magnesium sulfate?	
#23	Section 3.1.7 and beyond	te	Stoichiometry	Most calculations here are based on stoichiometry. While there are good reasons for this, are there some limitations that may make calculation results not reflect realistic practice, so that a margin could be given to avoid underestimation of inputs?	
#24	Section 3.1.8	te	Electricity supply	See comments above. Is a global supply of electricity warranted? Should it be European based? Were marginal mixes used?	
#25	Section 3.1.15	te	Assumption of abatement	Is this assumption realistic? Test it in sensitivity analysis?	
#26	Section 3.2	te	Old data used as reference	How representative is the Almeria plant of the system being modelled here? Geographically speaking, Almeria is not representative of Europe but perhaps this is irrelevant in this context.	
#27	Section 3.2.2	te	iLUC model	Why is land expansion only onto agricultural land? Could you give the factor used in terms of ha-yr as well? I suspect that the conversion will give an extremely high number. In Table 27: if we have 300g CO2 per kg NPP0, an average European ha of 6000kg NPP0 as C would incur 1.8t CO2? The last version of the iLUC user manual I have (4.1 from 2014) gives a factor of 1.26 t CO2/pw ha*year, which is about 2/3 of 1.8tCO2.	
#28	Section 3.3.6	te	Linear extrapolation	This makes sense if there is no reason to believe otherwise, but is there a case for non-linear extrapolation?	
#29	Section 3.4.2	te	Ecoinvent dataset for steel	Was the original dataset modified to reflect a waste treatment activity?	
#30	Section 3.5	te	Realism of assumption	Is it reasonable to assume that the plant operates 365 days per year?	
#31	Section 3.6	te	Double counting	Combustion excluded from steam cracking. Please see comments above and ensure the two systems under comparison are modelled consistently and reasonably.	

1st iteration: itemized reply by 2.-0 LCA consultants

Itemized reply to the Critical review report of the study: "Life cycle assessment of the LICROX technology"

By Ivan Muñoz
2.-0 LCA consultants, Barcelona, Spain
24 May 2022

Background

This document presents an itemized reply to the comments and suggestions made in April 2022 by the reviewer, Dr. Miguel Brandão, to the study "Life cycle assessment of the LICROX technology", dated 24 March 2022, which reports on the goal and scope definition and life cycle inventory (LCI) phases of the life cycle assessment (LCA) study.

I thank the reviewer for his positive feedback and constructive comments.

Itemized reply

Below we list the 31 comments made by the reviewer and the corresponding replies as well as actions taken regarding the report and/or the model.

1. ***Wrong choice of word?: Replace "fabricate" with "produce". "Fabricate" is usually used in the context of producing misleading and inaccurate data.***

This has been changed as suggested.

2. ***The scope may have been exaggerated: Can the study really say whether the LICROX technology is sustainable or not? Will a cost assessment be carried out?***

I have replaced the term 'cost-effective' by simply 'effective'. As the reviewer suggests, this LCA study will not involve a parallel cost assessment.

3. ***CO2 as a by-product: Is CO2 clearly a by-product? I think this is always the case but a justification may be warranted and, if not, results could be tested for their sensitivity to considering CO2 differently.***

I have added a reference justifying the identification of CO_2 as an industrial by-product:

Pierantozzi R (2003) Carbon Dioxide. In: Kirk-Othmer Encyclopedia of Chemical Technology. Wiley. DOI: 10.1002/0471238961.0301180216090518.a01.pub2.

This reference has also been added in section 2.10.1, where CO_2 as an industrial by-product is also discussed.

In its introduction, Pierantozzi et al. (2003) state: "*Today carbon dioxide is a by-product of many commercial processes: synthetic ammonia production, hydrogen production…*".

4. ***Substitution: This is indeed the correct approach for a consequential LCA. A clear list of all marginal products that are assumed to be displaced (as well as their inventory) would be welcomed.***

All substituted products are identified and quantified in section 3 (inventory analysis).

5. ***Figure 3 excludes by-products (and substituted product systems): Include main by-products and product systems displaced by these.***

Figure 3 has been modified to include substituted products. This affects the end-of-life stage only. The number of substituted products is quite numerous due to the recycling activities (steel, aluminium, copper, glass, heat, electricity, gold, silver, palladium…). In the figure it is not practical to show all individual products, so we focus on the main ones instead (steel, aluminium, glass). The rest are shown as 'other'.

6. ***Given that Europe is the focus geographical unit, why use global averages here?: Consider whether or not it makes sense to use a European based average for the parameters currently using a World average ("average global scenario") for the supply of underlying materials.***

The reason for considering a global instead of a European supply scenario for the underlying materials is based on the fact that many of these materials, such as chemical precursors, etc., are expected to be traded in the global market, and so ideally a global marginal supply mix should be used. In practice, though, defining marginal supply mixes for a plethora of chemicals is not feasible given the time and resources available for this study. A global average approach seems the second-best approach available.

I have added this discussion in section 2.7.2. for better clarity.

7. ***Reference system: consistency with the system boundary of LICROX: Ensure that the delimitation of the system boundary in both system (LICROX and that representing ethylene produced from steam cracking) is consistent.***

When the model for petrochemical ethylene is compared to that of LICROX, the main consistency issue was the mass allocation approach used for petrochemical ethylene. Now a fully consequential model has been elaborated in the revised report for petrochemical ethylene.

8. ***Issues of scale: Given that a not even a LICROX prototype exist, scaling is indeed challenging (as identified). Could a certain % increase in efficiency be assumed to reflect an established level of production?***

We have tried to cover the scale issue as best as possible. Sometimes this even involves forgetting about the currently available data altogether, and finding a suitable proxy, rather than using what the consortium provides. As an example, the prototype is expected to use 0.5 kW to power auxiliary devices for 100 cm^2

PEC. This means 50 kW/m^2 or 6,667 kWh/kg ethylene (assuming 10 h operation/day and the yield of 0.075 kg/m^2/day). The figures are so far off in cases like this that a % increase in efficiency is simply not enough, as we are talking about orders of magnitude. For this reason, it is sometimes more appropriate to use a proxy technology, like the considered photocatalysis plant. I hope we have better data for the second iteration, allowing us to fill at least part of the gaps.

9. ***Efficiency assumptions: It may be optimistic to assume 100% efficiency in e.g. the subsequent sections as well use of CO2 and water.***

I have consulted with the consortium on this. They suggest that the actual utilization efficiency could be as low as 8%, and that for this reason CO_2 will need to be recirculated. When recirculation is taken into account, the CO_2 losses are expected to be minor, but actual figures are not available. As a default scenario we still consider 100% efficiency in the study. These assumptions are now mentioned in section 3.3.1 (carbon dioxide).

10. ***How would the assumption of atmospheric CO2 affect the results (if at all)?***

According to the consortium, using atmospheric CO_2 is currently not an option, given that there are no catalysts that can work at such low CO_2 concentrations. Such an option, if feasible, would certainly improve the overall life cycle impact. For the second iteration, the consortium has expressed interest in assessing a scenario where CO_2 is directly supplied from flue gases in the vicinity of e.g. a power plant.

11. ***Plant dismantling operation excluded: I trust the reference steam cracking plant dismantling operation is also excluded?***

This is a good question as I did not explicitly look at this. The answer is yes, it is included as part of the ecoinvent data set for an organic chemicals factory. It includes construction and dismantling.

12. ***Ecoinvent version 3 system model: Perhaps mention here that the ecoinvent system model of Ecoinvent is used?***

It is now mentioned, as suggested.

13. ***Consistency in how the two systems under comparison are modelled: I understand that the data from Franklin associates is used for the steam cracking model. But this system is delimited with reference to mass allocation, which may render it incomparable with the LICROX system under assessment.***

I am aware of this limitation. I have now been able to replace the US LCI data set for petrochemical ethylene by a fully consequential model, built based on data reported by Rodríguez-Vallejo et al. (2020). This makes for a consistent comparison of both LICROX and petrochemical ethylene.

Reference:

Rodríguez-Vallejo DF, Guillén-Gosálbez G, Chachuat B (2020) What Is the True Cost of Producing Propylene from Methanol? The Role of Externalities. ACS Sustainable Chemistry & Engineering 2020 8 (8), 3072-3081.

14. ***Consistency in the state of-the-art of different impact categories: Stepwise 2006 is used with updates on some categories. Given that the method was developed 15 years ago, can you justify the choice of adopting it, especially in light of having only some, not all, impact categories updated, which may bring an issue of inconsistency. Furthermore, can you include a justification of why the hierarchist approach in ReCiPe 2013 was adopted?***

I am aware some parts of Stepwise can be considered outdated. The main reason why we choose to use Stepwise over other more recent impact assessment methods is because of its unique approach to weighting through monetarisation. We have now stated this in the text.

Regarding ReCiPe, perhaphs there is a confusion, since we do not rely on ReCiPe for any of the impact categories.

Also, we include now in the final first iteration report an additional impact assessment calculation with an alternative method, namely ILCD2011+, which is available in SimaPro. At the mid-point level, both methods result in very similar relative results.

15. ***CO2 source and C sink Missing environmental mechanism? See above. Is the timing of sequestration and emissions of GHGs accounted for in the sense that earlier flows have a larger GWP? I do not think that it is, but the iLUC model implicitly does this, so there may be an issue of consistency. The consideration of the CO2 input could be excluded if no differentiation vis-à-vis timing of emissions is made. If it is made, several methods exist that account for this. How is temporary carbon storage in landfills dealt with, if at all? Also, make sure that having a cradle-to-gate approach does not make the comparison erroneous and mass imbalanced.***

Temporary storage of carbon in ethylene per se is not attributed any environmental benefits. What is credited, in the case of LICROX, is the fact that biogenic carbon is being stored instead of fossil (regardless of the time of this storage). Regarding landfilling, if carbon from LICROX ethylene was being landfilled, and this carbon was embedded in non-degradable materials, such as polyethylene, this could be considered as a carbon sink. But this sink is precisely what we are crediting to LICROX already, that is -3.14 kg CO_2/kg ethylene. If we were doing a cradle-to-grave LCA of LICROX ethylene used to make polyethylene, and this material was sent to landfill at the end-of-life stage (EoL), then the credit of -3.14 kg CO_2 would be found at EoL instead of at the gate of the LICROX plant, but we end up with the same credit in both cases. Essentially, by crediting at the gate of the LICROX plant what we are doing can be understood as a form of system expansion.

16. ***iLUC: Define the term here?***

The term is in fact defined in the second line of section 2.10.2, the first time it appears.

17. ***iLUC does not assume only deforestation, as e.g. grassland is also part of the land supply mix. Referring only to deforestation may be misleading.***

In the particular case of the market for arable land, as modelled by Schmidt et al. (2015), productive capacity is supplied only from land intensification and from expansion, the latter referring to deforestation. Land covered with grass, which is fit for arable cropping is part of arable land. A change in demand for arable land does not affect conversion of land covered with grass into cropland.

18. ***iLUC: NPP0 refers to potential NPP***

Correct. It has been changed in the text.

19. ***"unspecified European country": What does this mean? Is it representative of the European (weighted) average?***

This means the PEC is likely to be produced in Europe, but we do not know where. I have added in the text a sentence explaining this means that in the model this is included as an average European production scenario.

20. ***Missing data: I understand that data may not exist to characterize such a novel technology. Some of these data are expected to be made available for the second iteration, but the level of "guesstimating" in this study is extremely high.***

I agree. I do not see any way around this, though, at least for this first iteration.

21. ***Double counting: See comments above. It is important to make sure that CO2 accounting is consistent with the goal and scope and with the systems' delimitations.***

Accounting for CO_2 emissions from solvent degradation in the atmosphere ensures a complete picture of the greenhouse-gas emissions of PEC manufacturing. If these solvents would instead be sent for incineration, it would be expected to count conversion of the solvents to CO2 through combustion. The difference in this case is that with solvent evaporation, the conversion to CO2 does not happen in the technosphere, but in the ecosphere. In principle, ecosphere processes are captured by impact assessment methods and not in the inventory, but global warming potentials (GWP) do not cover this aspect. Thus, we have two solutions if we want to account for these emissions: we either 1) calculate a GWP for each solvent, that expresses the amount of CO_2 indirectly generated from its degradation in the atmosphere, or 2) we include these CO_2 emissions as part of the inventory, even though this has the drawback that solvent emissions are counted once as solvents (which contribute to e.g. respiratory organics, toxicity…) and again as CO_2. We opted for approach 2. In practice both solutions lead to the same end result.

22. ***Missing data: See comments above. I understand data may not exist for all activities. Several approximations had to be incurred in throughout the study. In this section, is lead a good***

approximation for bismuth? Are data for vanadyl sulfate acceptably similar to that of magnesium sulfate?

Regarding bismuth, the problem is not only that there are no data in ecoinvent, but also that bismuth is mainly obtained as a by-product from mining other metals. According to Ibn-Mohammed et al. (2018): “bismuth is primarily obtained as a by-product of lead and copper smelting and sometimes from tin, tungsten and zinc ores from China”. Thus, an increase in demand for bismuth is not likely to drive an increase in supply. Lead and bismuth are actually quite close chemically. In fact, bismuth seems to be replacing lead in many applications according to the same authors, so it is perhaps not so far-fetched to assume lead is affected by changes in demand for bismuth. In any case, it is not feasible to create life-cycle models from scratch for all materials we don’t find in ecoinvent. As a matter of fact, we are already doing that as we have created inventories for at least 10 materials we did not find in ecoinvent.

Regarding vanadyl sulfate, the situation is similar. It is simply not practical to create ad-hoc inventories for all chemical precursors involved, and this is a good example. We need data for vanadyl acetylacetonate, which is not available in ecoinvent. So, we decided to create an inventory for it. It turns out that it involves an input of vanadyl sulfate, which is not in ecoinvent either. So, we decided to create an inventory for it. It turns out that vanadyl sulfate requires inputs of vanadium, but this is not available either. We could then try and create an inventory for vanadium. We could go on like this forever.

Given the uncertainties and data gaps involved, it is clear that in this study we can only aim at getting the order of magnitude right. If we achieve that, we should be happy.

Reference:
Ibn-Mohammed T, Reaney IM, Koh SCL, Acquaye A, Sinclair DC, Randall CA, Abubakar FH, Smith L, Schileo G, Ozawa-Meida L (2018) Life cycle assessment and environmental profile evaluation of lead-free piezoelectrics in comparison with lead zirconate titanate, Journal of the European Ceramic Society, 38 (15): 4922-4938.

23. ***Stoichiometry: Most calculations here are based on stoichiometry. While there are good reasons for this, are there some limitations that may make calculation results not reflect realistic practice, so that a margin could be given to avoid underestimation of inputs?***

Our approach is not so different to that used in the ecoinvent database whenever data are not available, namely stoichiometry and a yield of 95% in chemical reactions. This is stated in Hischier et al. (2005), describing the approach used in version 2 of the database for chemicals with “very weak data availability”. It is our opinion that assuming 95% over 100% efficiency mostly leads to complicating calculations and little extra benefit, and for this reason 100% was chosen.

Reference:
Hischier, R., Hellweg, S., Capello, C., Primas, A. 2005. Establishing Life Cycle Inventories of Chemicals Based on Differing Data Availability. The International Journal of Life Cycle Assessment.10 (1), 59-67.

24. Electricity supply: See comments above. Is a global supply of electricity warranted? Should it be European based? Were marginal mixes used?

This has been partly addressed in comment #6. The global electricity supply data set in ecoinvent is meant to reflect marginal supply, as we are using the consequential system model in this database.

25. Assumption of abatement: Is this assumption realistic? Test it in sensitivity analysis?

I do not have a reference to back up this assumption, but unless this is abated, the process would have huge SOx emissions. Ironically, it turns out molybdenum trioxide is included in ecoinvent, but I have only realized this after having created this dedicated inventory. In practice ecoinvent also more or less developed their model based on stoichiometry, etc., and they also consider SOx abatement. The ecoinvent LCI reports 0.0623 kg SO2/kg MoO3, while in our model we estimate 0.089 kg SO2/kg MoO3, which is very close.

26. Old data used as reference? How representative is the Almeria plant of the system being modelled here? Geographically speaking, Almeria is not representative of Europe but perhaps this is irrelevant in this context.

We are using this reference mainly as an approximation for:

- Land use
- Infrastructure
- Energy use for auxiliary devices

We received feedback from one of the partners (ICFO) stating that this approach sounds reasonable in the absence of better data at this point. As pointed earlier in the review, given the involved uncertainty at this stage, this is seen only as a means to obtain a complete inventory, that more or less gets the orders of magnitude right.

The use of Almeria would be inappropriate if we used it to obtain very location-specific aspects, such as solar energy resources, which are much higher in Almeria than the European average.

27. iLUC model: Why is land expansion only onto agricultural land? Could you give the factor used in terms of ha-yr as well? I suspect that the conversion will give an extremely high number. In Table 27: if we have 300g CO2 per kg NPP0, an average European ha of 6000kg NPP0 as C would incur 1.8t CO2? The last version of the iLUC user manual I have (4.1 from 2014) gives a factor of 1.26 t CO2/pw ha*year, which is about 2/3 of 1.8tCO2.

Cropland is usually flat, easily accessible and close to urban areas, so it is more attractive for industrial expansion than let’s say hilly forest land. We have found data backing this up in the particular case of China, stating that between 1990 and 2015, industrialization has led to the loss of 1.76 million hectares of cropland (Zhang et al. 2021). We have added this in the text (in section 2.10.2).

About table 27, the reviewer is spot on, as the numbers are erroneous. Fortunately, the errors are in the report only, and not in the model. The right figures are, per kg NPP_0:

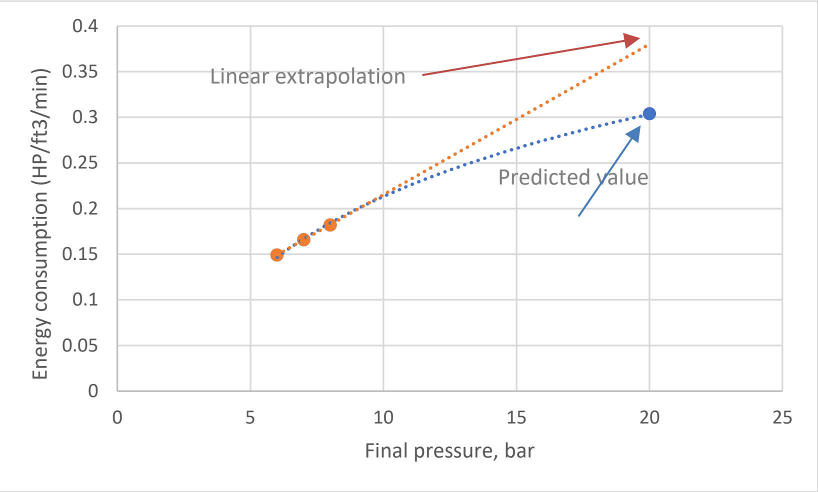
- N fertiliser: 0.0096 kg
- Ammonia: 1.15E-03 kg
- Dinitrogen monoxide: 2.21E-04 kg
- Nitrogen oxides: 5.56E-05 kg
- Nitrate: 0.0142 kg
- Occupation, accelerated denaturalisation, secondary forest to arable: 0.539 m^2-yr
- Carbon dioxide: 0.18 kg

These figures have been inserted in table 27.

Reference:
Zhang C, Kuang W, Wu J, Liu J, Tian H (2021) Industrial land expansion in rural China threatens environmental securities. Front. Environ. Sci. Eng. 15 (2):,29.

28. Linear extrapolation: This makes sense if there is no reason to believe otherwise, but is there a case for non-linear extrapolation?

I have made an additional search on this subject. Engineering toolbox[2] offers a formula to calculate energy use for air compression, that shows that the relationship is not exactly linear, but almost. In the figure below I used their formula to plot energy use (Horsepower/ft^3/min) vs. pressure, for four pressure values. The predicted value at 20 bar is 0.3 HP/ft^3-min or 0.133 kWh/m^3 air. Engineering ToolBox suggests adding +20% to account for friction losses, so this would make it 0.16 kWh/m^3. If we make a linear extrapolation from the values for 6,7, and 8 bar to our target value of 20 bar, this leads to 0.37 HP HP/ft^3-min or 0.195 kWh/m^3 air (after adding +20%). So, a linear extrapolation slightly overestimates energy use.



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[2] https://www.engineeringtoolbox.com/horsepower-compressed-air-d_1363.html

In the study what we did was to take the energy consumption figures from ecoinvent for 6, 7 and 8 bar, and use these to extrapolate linearly to 20 bar, leading to 0.4 kWh/m^3. As seen in the graph, a linear extrapolation is likely to lead to an overestimate of the energy use, but the relative difference is reasonably small. The question that remains is whether to rely on the Engineering Toolbox formula to predict the energy use (leading to 0.195 kWh/m^3) or to stick to the ecoinvent linear extrapolation (0.4 kWh/m^3), even if the latter slightly overestimates the value. I have opted to stick to the ecoinvent extrapolation, the reason being that the underlying values in ecoinvent are based on actual industrial compression plants, rather than on a theoretical calculation.

A comment has been added in the text stating that we are likely to be slightly overestimating the energy consumption.

29. ***Ecoinvent dataset for Steel: Was the original dataset modified to reflect a waste treatment activity?***

The data set has not been modified. Only the sign is reversed. This data set is used with a positive sign for example by steel production data sets, to reflect an input of steel scrap. It is also used with a negative sign (as we do here) to refer to recovered waste. This is done for example by waste incineration data sets, where steel scrap is recovered from the slag.

30. ***Realism of assumption: Is it reasonable to assume that the plant operates 365 days per year?***

I have discussed this with the consortium, but they do not have a very clear idea. A partner suggested the plant working from Monday to Friday, but just because this is what they foresee for their prototype. In the LCA, however, we do not want to reflect how a prototype operates, but a commercial plant, which I would assume would not stop for the weekends. In the end, the consortium agreed to use a figure of 90% of useful operating time. This value 90% is taken from a study evaluating a hypothetical industrial PEC plant in the United States (Sathre et al. 2014). This is now included in the model and mentioned in section 3.5.

Reference:
Sathre R, Scown CD, Morrow WR, Stevens JC, Sharp ID, Ager JW, Walczak K, Houle FA, Greenblatt JB (2014) Life-cycle net energy assessment of large-scale hydrogen production via photoelectrochemical water splitting. Energy Environ. Sci., 2014,7, 3264-3278.

31. ***Combustion excluded from steam cracking. Please see comments above and ensure the two systems under comparison are modelled consistently and reasonably.***

Combustion of fuels for steam cracking was included either as direct emissions reported by Franklin Associates, or in the fuels data sets themselves. Care was taken to make sure that we did not double count emissions (as direct emissions and in fuel data sets). In any case, this data set is no longer used, as explained in comment #13.

Regarding the carbon in ethylene, as it has already been explained, the carbon stays in the molecule, as this is a cradle-to-gate study. The fact that LICROX incorporates carbon that would otherwise have been emitted to the atmosphere is included as a credit of -3.14 kg CO_2/kg ethylene.

2nd iteration: reviewer comments and final review statement

Critical review report and statement of the study:
“Life cycle assessment of the LICROX technology”
By Miguel Brandão, PhD
21st November 2022

1. Introduction

The present document reports the review made to a life cycle assessment (LCA) study of the LICROX technology. The LCA study in question (Muñoz, 2022) was performed by Ivan Muñoz, from 2.-0 LCA consultants, and commissioned by the EU-funded HORIZON2020 project consortium, under which the LICROX technology is being developed. This is the revision of the second iteration, sent on 24th October, and sent back on 21st November.

LICROX is a scientific project in which photoelectrochemical cells are being developed to mimic natural photosynthesis and allow for a sustainable formation of ethylene. As part of this project, an LCA of the LICROX technology will be conducted to estimate its impacts on 16 environmental categories (following the stepwise method).

The LCA study reviewed consists of the second iteration related to the definition of scope and life cycle inventory. Furthermore, results are estimated for the distribution of 1 kg of ethylene, and compared with a more traditional way of producing ethylene (i.e. steam cracking).

2. Scope of the review

This review characterises the study against a fixed set of criteria that are commonly used in LCA reviews and can be found in the ISO standard 14071 (ISO, 2014). These characteristics cover each of the four phases of LCA, and this review is structured around those: 1) goal & scope definition, 2) inventory analysis, 3) impact assessment and 4) interpretation.

This critical review ensures that the methods used to carry out the LCA are consistent with the ISO standards - 14040 (ISO, 2006a), 14044 (ISO, 2006), as well as technical specification (TS) 14071 (ISO, 2014) – and are scientifically and technically valid. It also ensures that the data used are appropriate and consistent with the goal and scope of the study. Finally, this review ensures the LCA report is transparent and consistent. All these features are required by TS14071 (ISO, 2014) and represent the checks and balances that ensure the quality of the study.

This review is performed based on expert review. It has been performed at the end of the study, and no changes are expected to occur after the production of this report, which represents the final stage of the 5-stage procedure:

1. Reviewer reads and comments on the report
2. Study authors will go through reviewer comments one by one and make a revised report and an itemized reply
3. Reviewer reads the authors’ itemized reply and give any potential remaining comments
4. Authors will go through any remaining issues the reviewer might have and make a revised LCA report and itemized reply

5. Reviewer reads author’s revised itemized reply and makes final review statement (applicable only to the final iteration).

This review report corresponds to step 5 above and pertains the second and final iteration. It excludes a detailed assessment of the life cycle inventory (LCI) model and of the individual data sets but, as required by TS14071 (ISO, 2014), it covers all aspects of the LCA’s definition of scope and life cycle inventory (LCI), including data appropriateness and reasonability, calculation procedures and calculated LCI results, as well as life cycle impact assessment (LCIA) and interpretation.

It is outside the scope of this review to address the goals chosen for the LCA study in question, as it is impossible to either verify or validate them. The responsibility for those, as well as the ways in which the LCA results are used, lie with the commissioner of the LCA study. Specific comments to the definition of scope and life cycle inventory study were sent during the last iteration, and all comments were addressed satisfactorily. The adjustments made to Figure 3 seemed not to have made it to the final version, however.

3. Review of LCA study of the LICROX technology

3.1. Goal and scope definition

LCA practice is standardised by the International Organization for Standardisation (ISO) in ISO14040 (ISO, 2006a) and ISO14040 (ISO, 2006b). These standards include the terminology and requirements for LCA studies, such as the process for conducting LCA studies, methods, data, evaluation, documentation, etc. ISO compliance ensures that the study adheres to those internationally-agreed rules and, thus, credibility and bias-freedom. However, it may not necessarily ensure scientifically soundness and robustness.

This section of the study covers an explanation of what this particular stage is and where it falls within the four phases of an LCA. It also includes a description of the process of the: critical review, purpose (including data collection, temporal and geographical scope), functional unit, life cycle inventory model and life cycle impact assessment (including the adopted environmental impact categories, as well as how biogenic emissions and indirect land use were dealt with), system boundaries and reference flows (which were clearly specified).

The following has been verified:

- The study under review claims to be compliant to the above standards. This is indeed attested.
- It is specified that the study will go through a critical review.
- The study’s goals are clearly formulated, as are the intended application and audience.
- Data collection follows concerns of consistency.
- The temporal scope is specified.
- The geographical scope is delimited to Europe for the foreground system, while inputs to the foreground come from the rest of the world in an average-global manner.
- The functional unit is specified and is appropriate. It will be used for comparison purposes.
- It is clearly stated the LCI model follows a consequential approach and an explanation of the approach is given.

- It is clearly stated that the LCIA method used is Stepwise 2006 and an explanation of the method and updated are given. A comprehensive set of environmental impact categories was adopted and identified.
- Treatment of biogenic carbon and methane is explained and justified properly.
- Nature occupation is modelled consistently with that of iLUC.
- System boundaries delimitation: cut-off as Input-Output databases are not used. The exclusion of the use-phase and of the end-of-life phase is justified and correct.

3.2. Life cycle inventory (LCI)

This section describes the data and modelling in the reviewed LCA study. It starts by making a distinction between the foreground and background systems. Subsequently, it explains the use of ecoinvent for the background data, and a general description of that database. The consequential system model version used ensures consistency with the consequential approach.

Indirect land use changes (iLUC) – which are often neglected in LCA – are modelled in a consistent way with the rest of the LCA model.

Other general activities related to production (photoanode, photocathode, OPV), infrastructure, inputs (electricity, chemicals and water), plant (operation and disposal) and wastewater treatment, are described appropriately. Care was taken to avoid inappropriate double-counting.

The involved activities are described and inventory summaries shown, including photoelectrochemical cell manufacturing, plant infrastructure, operation, disposal, as well as those related to the alternative way of producing ethylene: steam cracking.

3.3. Life cycle impact assessment

A very competent LCIA, included weighting via monetarisation as per the Stepwise method, is applied and its results shown, including a contribution analysis for 16 midpoint impact categories, in terms of both dominant emissions and hotspots. A more detailed contribution analysis is made on global warming and respiratory inorganic impacts.

It is shown that the new technology appears to be worse in all environmental impact categories but one, which is an interesting finding.

3.4. Interpretation

The study includes sensitivity, completeness and consistency checks. Furthermore, limitations are identified. Results are discussed, as are reasons for the results. The conclusions extrapolated are robust and rest on the analysis reported that preceded it.

4. Conclusions

The review of the LCA study on the LICROX technology revealed an extremely competent analysis that underwent the rigorous application of the aforementioned ISO standards. Thus, it can be inferred that the both parts of the study reviewed are ISO-compliant, consistent and scientific applications of the LCA methodology.

Given the infant nature of this technology, and associated inexistent of specific data, the author went into great lengths to ensure the best possible representativeness of the data used. Robust-enough approximations were used throughout the study, which only attests to the high competence of the study.

I therefore conclude that the study made is of high quality, and can support environmental decision making.

Miguel Brandão

Miguel Brandão, PhD
Associate Professor in Industrial Ecology and Life Cycle Assessment
Department of Sustainable Development, Environmental Science and Engineering (SEED)
KTH - Royal Institute of Technology

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CV Dr. Miguel Brandão

Dr. Miguel Brandão is Associate Professor in Industrial Ecology and Life Cycle Assessment at KTH, Stockholm. Over the last 17 years, he has taught and researched at a number of organisations around the world. He works with the use of hard systems approaches that can robustly support decisions towards sustainable development. His research has focused on the integrated assessment of bio-based systems, with emphasis on their impacts on climate change, resource depletion, ecosystem services and biodiversity. He was/is involved in international standardisation initiatives (PAS2050, ILCD, FAO LEAP, ISO, GHG Protocol) in the areas of life cycle assessment, carbon footprinting, circular economy and climate-change metrics. He is the coordinator for research and innovation in circular economy at KTH, and also KTH's academic responsible for Latin America in the areas of student recruitment, exchange studies, and business and research collaboration. His interests include: Circular Economy, Environmental Economics, Ecological Economics, Agroecology, Land Use, Sustainable Production and Consumption, Globalisation, Poverty alleviation, Food Security, Bioenergy, Food Systems. He is associate editor in the Journal of Industrial Ecology (LCA), the International Journal of Life Cycle Assessment (Land Use), Sustainability (Social Ecology and Sustainability), Clean Technologies, Frontiers in Climate (Negative Emissions Technologies) and Standards. In 2012, he received the SETAC Europe Young Scientist LCA Award.