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METHODS ARTICLE

PULPO

A framework for efficient integration of life cycle inventory models into life cycle product optimization

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Abstract

This work presents the PULPO (**P**ython-based **u**ser-defined **l**ifecycle **p**roduct **o**ptimization) framework, developed to efficiently integrate life cycle inventory (LCI) models into life cycle product optimization. Life cycle optimization (LCO), which has found interest in both the process systems engineering and life cycle assessment (LCA) communities, leverages LCA data to go beyond simple assessments of a limited number of alternatives and identify the best possible product systems configuration subject to a manifold of choices, constraints, and objectives. However, typically, aggregated inventories are used to build the optimization problems. Contrary to existing frameworks, PULPO integrates whole LCI databases and user inventories as a backbone for the optimization problem, considering economy-wide feedback loops between fore- and background systems that would otherwise be omitted. The open-source implementation combines functions from Brightway2 for the manipulation of inventory data and pyomo for the formulation and solution of the optimization problem. The advantages of this approach are demonstrated in a case study focusing on the design of optimal future global green methanol production systems from captured CO_2 and electrolytic H_2. It is shown that the approach can be used to assess sector-coupling with multi-functional processes and prospective background databases that would otherwise be impractical to approach from a standalone LCA perspective. The use of PULPO is particularly appealing when evaluating large-scale decisions that have a strong impact on socioeconomic systems, resulting in changes in the technosphere on which the background system is based and which is often assumed constant in standard LCO approaches regardless of the decisions taken. This article met the requirements for a gold-gold *JIE* data openness badge described at http://jie.click/badges.

KEYWORDS
ecoinvent, industrial ecology, life cycle optimization, methanol, multi-scale, technosphere-wide

1 INTRODUCTION

1.1 Motivation

Life cycle assessment (LCA) (ISO, 2006) has recently gained much traction and has become pivotal for quantifying the environmental impacts of products and services, supporting decision-making in a wide range of sustainability problems (Hellweg & Milà i Canals, 2014; Sala et al., 2021). Notably, LCA is increasingly used to compare technology and material choices throughout a product's life cycle, for example, alternative sources of CO_2 and H_2 feedstocks and processing technologies for low-carbon chemicals production (Cuéllar-Franca & Azapagic, 2015; Galán-Martín et al., 2021), insulation materials in the construction of buildings (Schiavoni et al., 2016), solid waste materials for use in highway pavement construction (Li et al., 2019), and plastic waste management solutions (Alhazmi et al., 2021).

LCA on its own answers critical questions such as "Which production alternative performs environmentally better?" or "Which stage of a product's life contributes most to its environmental impact?" In addition to these fundamental questions, amid stringent sustainability targets such as the Paris Agreement 1.5°C target, there is an urgent need to identify optimal product systems that yield the highest environmental benefits considering a range of alternative technologies and associated locations. However, the products supply chain may involve hundreds of technology choices, which, along with regional and temporal variability and system constraints (e.g., resources availability and production capacity), makes the determination of the most environmentally appealing scenario a major challenge.

The idea of integrating LCA and optimization dates back to the pioneering work of Azapagic and Clift (1999), who proposed integrating LCA and linear programming. This so-called life cycle optimization (LCO) framework addresses subsequent inquiries like "How can we redesign a product's supply chain to minimize environmental impacts, meeting technical and systemic constraints and targets?" For a detailed review of studies related to process optimization, we refer the reader to Pieragostini et al. (2012) and for a more recent review of sector-specific integrated optimization frameworks to Ferdous et al. (2023). Most notably, LCO has found applications within the process systems engineering (PSE) community, where the underlying optimization models require an advanced degree of modeling and case study-specific expertise. Efforts were undertaken in the LCA community to integrate optimization approaches. However, the landscape of LCO frameworks and tools, while rich and varied, exhibits certain methodological and implementation limitations that have hindered their widespread adoption, especially by LCA practitioners.

1.2 Existing life cycle optimization frameworks and tools

The analysis of existing LCO frameworks and tools reveals a dichotomy between PSE-oriented tools and those with an LCA focus (Table 1).

PSE-oriented tools and frameworks, such as the ones developed by Sun et al. (2023), Zhao and You (2021), and Reinert et al. (2022) (SecMOD), offer advanced multi-scale (i.e., systems of different sizes and scopes) and multi-objective functionalities and sector-specific optimizations, but they require advanced expertise in process modeling. Moreover, they do not adhere strictly to the nomenclature and computational structure of LCA (Heijungs & Suh, 2002). On the other hand, LCA-oriented tools like SwolfPy by Sardarmehni et al. (2022) and ECOPT^2 by Hung et al. (2022) strive to extend LCA's traditional boundaries and integrate optimization functionalities. However, these efforts still fall short in terms of broad applicability and ease of use, being too sector-specific or lacking detailed comprehensive guidance for adaptation to other case studies. ECOPT^2 promises a sector-independent framework, yet potential extensions of the model beyond the transport-focused case study are not straightforward, and the use of the tool as an open-source platform is limited. Conversely, SwolfPy excels in providing comprehensive documentation and is readily accessible. However, its focus is tailored to solid waste management, featuring specialized process models and objective functions.

In a seminal work, Duchin and Levine (2011) introduced the rectangular choice-of-technology (RCOT) model, a linear programming input–output model that allows multiple technology choices across the economic sectors of a region. The RCOT model was later adapted to the LCA structure by Kätelhön et al. (2016, 2020), resulting in the technology choice model (TCM). The TCM constitutes a sector-independent approach, general enough for LCA practitioners to apply optimization without the extensive prior knowledge required by the PSE-inspired works. However, this framework shows some limitations.

First, in its current formulation, it primarily addresses technology choices within the foreground system, as the optimization problem is crafted in a bottom-up manner, combining inventories and information from several sources. This has been exemplified in a series of case studies, including the chemical industry (Kätelhön et al., 2019), the plastics industry (Bachmann et al., 2023; Meys et al., 2021), plastics recycling (Cornago et al., 2021), and the agricultural sector (Larrea-Gallegos et al., 2019). Expanding its scope to encompass the entire background system could potentially enable technology choices across the entire supply chain, from raw materials extraction to end-of-life. While the potential extension of the TCM to the background system has been recognized previously (Kätelhön, 2020), it remains unexplored.

TABLE 1 Overview of life cycle optimization frameworks and tools.

	Background choices (*via LCI import*)	Sector-independent	Open-source availability	Indicator and environmental flow constraints	Targeted area
– (Zhao & You, 2021)	✗	✗	✗	✗	PSE
– (Sun et al., 2023)	✗	✗	✗	✗	PSE
SecMOD (Reinert et al., 2022)	✗	○	✓	✗	PSE
ECOPT[2] (Hung et al., 2022)	✗	○	✗	✗	LCA
SwolfPy (Sardarmehni et al., 2022)	✗	✗	✓	✗	LCA
TCM (Kätelhön et al., 2016, 2020)	○	✓	○	✗	LCA
PULPO (**This work**)	✓	✓	✓	✓	PSE/LCA

Circles represent partially fulfilled aspects. Abbreviations: LCA, life cycle assessment; LCI, life cycle inventory; PSE, process systems engineering; PULPO, Python-based user-defined lifecycle product optimization; TCM, technology choice model.

While several extensions to the approach such as multi-objective (Budzinski et al., 2019) and multi-period (Zibunas et al., 2022) optimization have been proposed, to our best knowledge, additional constraints such as environmental flow constraints have not yet been implemented and studied before.

Another major limitation of the current state-of-the-art methods is the limited comprehensive demonstration of TCM's capabilities and flexibility, coupled with a lack of accompanying open-source implementation or software with detailed instructions and examples, which allows the methodology to be easily applied.

1.3 | Contribution

Here, we demonstrate the PULPO (**P**ython-based **u**ser-defined **l**ifecycle **p**roduct **o**ptimization) framework. PULPO can be used to find the best environmentally performing configuration of a product system considering all the stages in its life cycle. The main contributions of PULPO are as follows:

- From a methodological standpoint, the presented approach broadens the scope of TCM to include both foreground and background systems. It achieves this by transforming entire life cycle inventory (LCI) databases, along with user-generated inventories, in a top-down manner into a structured optimization problem. This innovative method allows for a thorough economy-wide evaluation of product systems. It enables the creation and resolution of optimization scenarios without the need to construct the entire system from scratch (bottom-up approach). Additionally, it leverages the wealth of data available in commercial LCI databases and can utilize inventories previously compiled by LCA professionals.
- From an implementation perspective, PULPO is designed to be easily accessible via its open-source implementation, fully integrated workflow in Python, and independence from commercial third-party software.
- Optional impact and environmental flow constraints, as well as lower supply bounds, have been implemented, allowing a more flexible specification of the system constraints.

PULPO is demonstrated in a case study focusing on sector coupling between the chemical and energy sectors via the manufacturing of methanol from captured CO_2. The global warming potential (GWP) reduction of synthetic green methanol deployment is assessed and optimized under three electricity-constrained climate change policy scenarios, utilizing prospective background databases generated via premise (Sacchi et al., 2022). Moreover, it is demonstrated how the approach handles the multifunctional process "power plant with carbon capture," which provides the main product, electricity, as well as CO_2. Two further motivating examples alongside extensive additional explanations can be found in Supplementary Information.

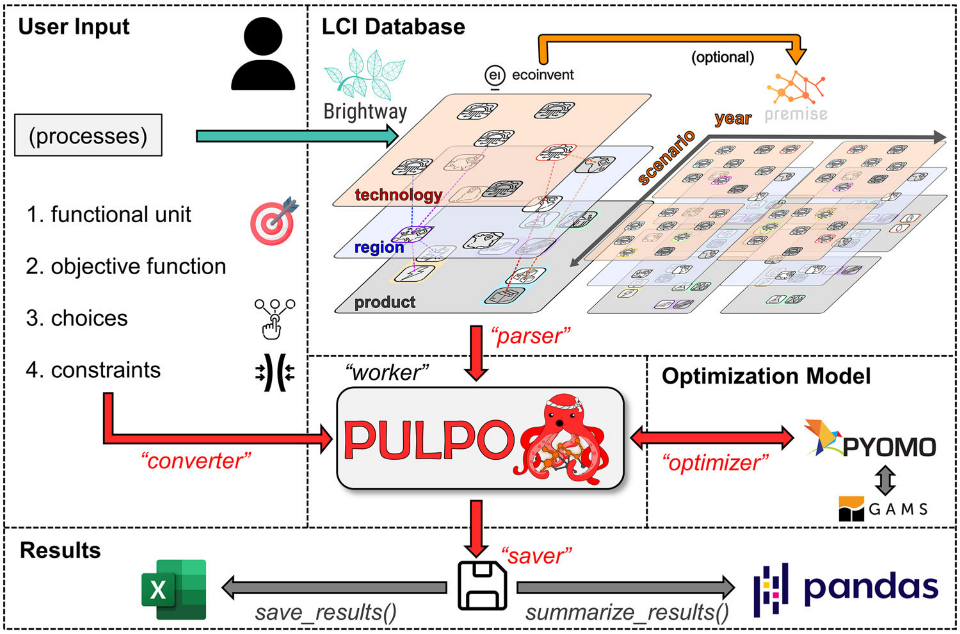


FIGURE 1 PULPO (Python-based user-defined lifecycle product optimization) information flow and connectivity to life cycle inventory (LCI) databases and other software packages.

The paper is organized as follows. Section 2 introduces the PULPO framework and its main capabilities. Section 3 demonstrates the use of PULPO in the sector coupling case study. Section 4 concludes this work and gives a perspective for the future use and development of PULPO.

2 | METHODS

2.1 | PULPO

Figure 1 illustrates the flow of information and the connectivity of the PULPO implementation to other software packages. It is openly available at Zenodo (Lechtenberg, 2023b) and GitHub. The main data input to the optimization problem is the technosphere matrix A, which is directly imported from sources such as ecoinvent (Wernet et al., 2016) or prospective background databases obtained from premise (Sacchi et al., 2022). LCA practitioners may introduce their own processes via Brightway2 (Mutel, 2017) or the Activity-Browser (Steubing et al., 2020). This technosphere matrix A then constitutes the backbone of the subsequent optimization tasks. It should be noted that using the entire LCI as a basis means that the results and conclusions hinge on the information contained within the selected database, as well as the data quality.

Once the data are collected, verified, and introduced into the database, the user must specify the optimization problem as follows:

1. **Functional unit**: The user specifies the functional unit through a Python dictionary that is indexed by the processes, assigning the final demand for the respective reference product. The process can be obtained from the database via the "*retrieve_activities*" function of the "*PulpoOptimizer*" class. This specification is mandatory for every LCA/LCO and describes the quantity of products (or functions) to be made available by the production system.
2. **Objective function**: The objective function is defined as the environmental impact category to be minimized. This can be set by the user via the "*methods*" argument when creating a "*PulpoOptimizer*" object. Life cycle impact assessment (LCIA) methods bundled with ecoinvent or premise may be utilized. In the code snippet of Table S1, the objective function is specified as "*('IPCC 2013', 'climate change', 'GWP 100a')*." Alternatively, custom sets of characterization factors, like those for the planetary boundaries method (Ryberg et al., 2018), may be incorporated.
3. **Possible choices**: In PULPO, the possible choices are sets of processes that provide equivalent products or functions. The user sets these choices through a nested dictionary that assigns a unifying label to the processes delivering equivalent products, which in turn have an upper capacity limit assigned by the user. This "*choices*" dictionary is then passed together with the "*demand*" dictionary to the "*PulpoOptimizer*" via the "*instantiate*" function. For example, if the functional unit is the production of 1 kWh of electricity, the subsequent user of this product may not distinguish if it has been produced from fossil or renewable sources, a turbine or a fuel cell, or in the neighborhood or another country. Thus, if the objective

is to supply this functional unit with minimal impact, these product-equivalent processes may be subject to **technology** and/or **regional** choices, as indicated by the different layers in Figure 1.

4. **Additional constraints**: Apart from the processes that are part of the possible choices, there is the possibility to set upper and lower bounds on every production process as a dictionary via the "*upper_limit*" parameter in the "*instantiate*" function. For example, the availability of raw materials, installed production, or storage capacities may be limited. Moreover, indicator and environmental flow constraints can be specified via the "*upper_imp_lim*" and "*upper_elem_lim*" parameters. Enforcing a minimum production level of a process is also possible via the "*lower_limit*" parameter. Further constraints may be added to expand the capabilities of PULPO.

PULPO takes these inputs and converts them into an optimization problem, which is implemented in pyomo (Bynum et al., 2021). The code snippet in Table S1 in the Supplementary Information presents a practical example. For details on the underlying mathematical model, see Sections S1 and S2. See also Section S3 for details on the introduction of slack variables to enable the specification of final production values (supply) instead of final demands. In its current form, the optimization problem may be solved using the commercial LP solvers included in the modeling and optimization platform GAMS (e.g., CPLEX), granted it is installed on the user's computer with a valid license, or, alternatively, the free and open-source solver HiGHS (Huangfu & Hall, 2018). The complexity of the final optimization problem depends on the dimensionality of the input as well as the specified degrees of freedom. The number of equality constraints corresponds to the number of processes modeled in the LCI database, plus the number of processes added by the user, minus the number of specified choices. To give the reader an idea of the base size of a commercial LCI database prior to adjustment and specifications by the user, the ecoinvent 3.8 cutoff system model database used in this work (Ecoinvent Association, 2021) has 19,595 processes (set j). In this list of processes, there are 7646 different technologies (unique process names), 300 regions, and 3392 products (i.e., unique reference products). The prospective background database obtained from premise (v1.6.7) for the SSP2-RCP1.9 scenario in 2030 has 30,026 processes. There are 4427 environmental flows (set e).

The PULPO workflow follows the ISO 14044 (ISO, 2006) phases, where the optimization part constitutes a repeated LCIA phase. Once the optimization is finished, the complete results can be saved in a spreadsheet. Moreover, a results summary can be displayed, focusing on the final impacts, the choices made, and the active constraints. This information should then be subject to the fourth and final phase of LCA, interpretation.

2.2 | Prospective background databases

Prospective LCA, according to the definition by Arvidsson et al. (2024), is an "*LCA that models the product system at a future point in time relative to the time at which the study is conducted.*" In that context, prospective background databases provide the necessary data to calculate the expected impacts of a modeled product or process when deployed at a future point in time.

RCPs (representative concentration pathways) are greenhouse gas concentration trajectories, and SSPs (shared socioeconomic pathways) are scenarios of socioeconomic development. Both are utilized within integrated assessment models (IAMs) to estimate the evolution of the economy and explore future environmental impacts. See Meinshausen et al. (2020) for further information on these concepts and Mendoza Beltran et al. (2020) for an explanation and demonstration of their importance in prospective LCA.

The use of prospective background databases is optional, but it enables users to diversify their assessments and potentially identify necessary conditions and limitations for the future deployment of new technologies. PULPO allows optimization of the foreground system, that is, to solve optimization problems where the specified choices include only the inventories added by the user in the foreground system like when optimizing the share of renewables in a power mix to be designed. However, the decision variables of the optimization problem might also belong to the background system, for example, when optimizing the fuel selection in the transportation activities employed to build the said power mix. We note that optimizing with the prospective background databases from premise (Sacchi et al., 2022) means that the resulting scenario deviates from the outputs of the IAM used to generate the initial prospective database. This discrepancy between the IAM and the PULPO results should be kept in mind when interpreting the results, as demonstrated later in the case study.

2.3 | Row elimination

Technosphere matrices A, like those provided by ecoinvent, have a characteristic structure. They are square ($j \times j$) where each process (column) corresponds to a single unique product (rows). The entries on the diagonal of that matrix are by default 1, while the rest of the entries are either 0 or negative. A negative sign of the element a_{ij} denotes that, to execute one unit of process j, the amount a_{ij} of product i is required as an input. Each column is scaled to one unit (kg, ton, m^2, …) of the reference product in the diagonal.

The A matrix below represents a simple example of a system that produces electricity via coal or wind power and a market that offers this electricity with an equal share. It can be seen how each process (column) corresponds to a unique product (row), indicated by the ones on the diagonal.

$$A = \begin{array}{c} \begin{matrix} \text{electricity market} & \text{coal} & \text{wind} \end{matrix} \\ \begin{pmatrix} 1 & -0.1 & -0.05 \\ -0.5 & 1 & 0 \\ -0.5 & 0 & 1 \end{pmatrix} \end{array} \begin{array}{l} \\ \text{electricity (from market) [kWh]} \\ \text{electricity (from coal) [kWh]} \\ \text{electricity (from wind) [kWh]} \end{array} \tag{1}$$

A standard LCA would determine the impact of 1 kWh of electricity supplied by the market. Mathematically, this implies solving the system of equations $A \cdot s = f$, for example, through inversion of the A matrix and subsequent multiplication with the demand vector f. The result of this can be seen below:

$$s = \text{inv}\,(A) \cdot f = \text{inv} \begin{pmatrix} 1 & -0.1 & -0.05 \\ -0.5 & 1 & 0 \\ -0.5 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1.08108 \\ 0.54054 \\ 0.54054 \end{pmatrix} \begin{array}{c} \text{electricity market} \\ \text{coal} \\ \text{wind} \end{array} \tag{2}$$

To supply 1 kWh of electricity from the market as a functional unit, the electricity market process must supply 1.08 kWh, which is higher than 1 kWh due to the self-consumption of electricity in the coal and wind power plants. To obtain the impacts, the scaling vector s must be multiplied by the biosphere matrix B and the characterization factors Q.

This system of equations is well-posed and A is square and non-singular, so its inversion is always possible. If the question to be answered is "Which is the (mix of) technologies supplying the electricity market, minimizing the GWP of 1 kWh electricity output of the market?" optimization should be considered.

In TCM, the construction of the rectangular matrix follows a bottom-up methodology. This entails assembling individual processes, represented as columns, sourced from diverse origins to form the composite matrix. In contrast, the row elimination method employed by PULPO follows a top-down approach. The rectangular technosphere matrix, here denoted as A^* $(i \times j)$, is obtained departing from existing LCI databases and user inventories by summing up the rows of products that are specified as equivalent choices (see Figure 2 for a conceptual illustration of the different approaches).

For the example above, this would mean that the rows "electricity (from coal)" and "electricity (from wind)" are summed up to form the new row "electricity*":

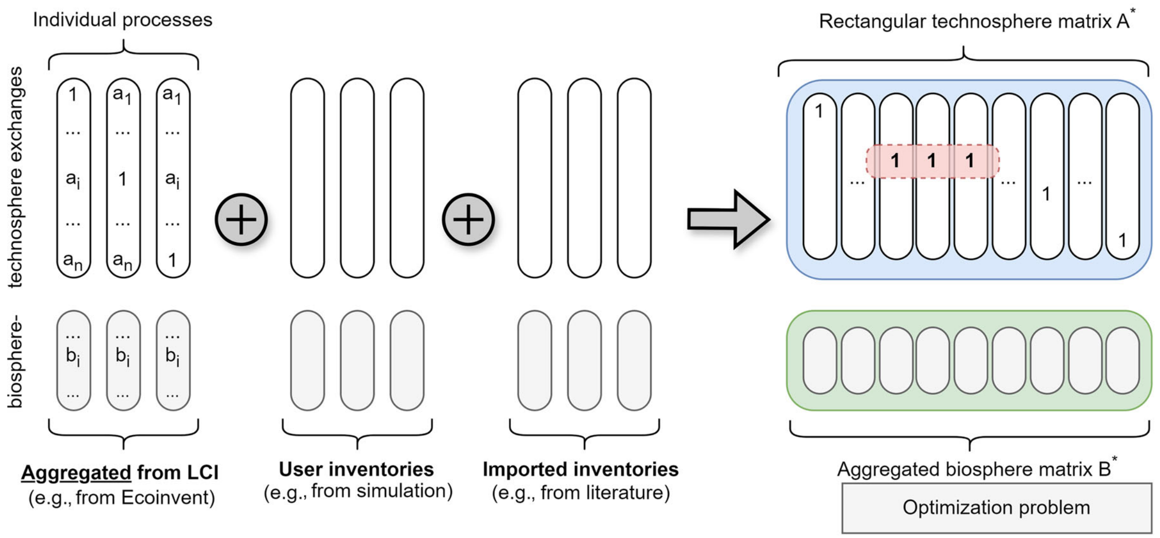
$$A^* = \begin{array}{c} \begin{matrix} \text{electricity market} & \text{coal} & \text{wind} \end{matrix} \\ \begin{pmatrix} 1 & -0.1 & -0.05 \\ -1 & 1 & 1 \end{pmatrix} \end{array} \begin{array}{l} \\ \text{electricity (from market) [kWh]} \\ \text{electricity}^* \text{ [kWh]} \end{array} \tag{3}$$

The resulting system of equations is underdetermined, so the solution to $A^* \cdot s = f$ is not unique anymore. Plugging this rectangularized matrix into the PULPO optimization problem and solving it yields the optimal values for s. They indicate the appropriate share of coal and wind power plants to the market, depending on the specification (objective, constraints …) made by the user. An exemplary resolution of this simple example is given in Supplementary Information S4.

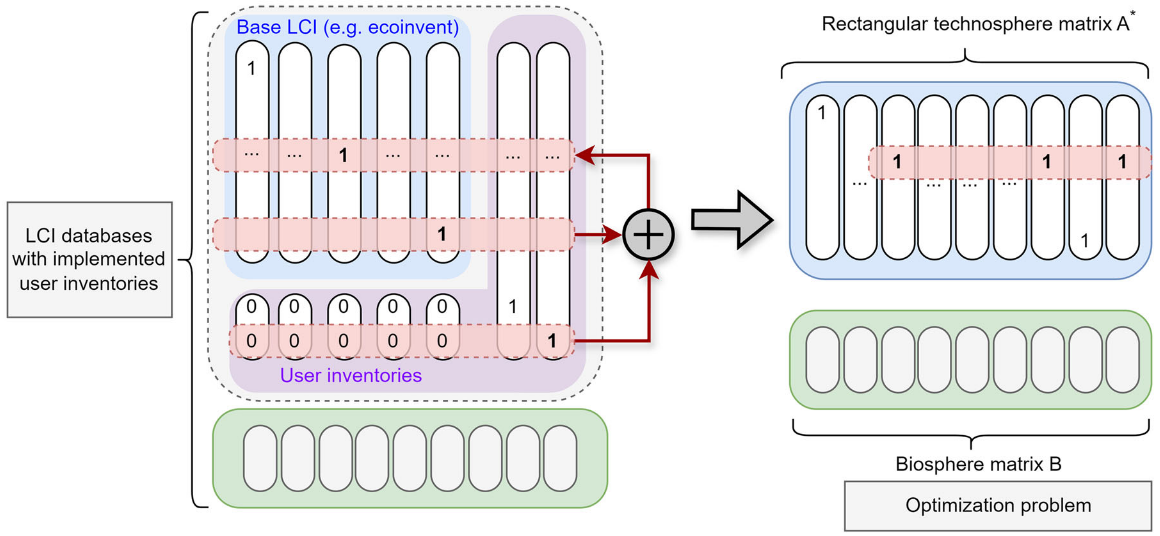
3 | DEMONSTRATION AND APPLICATION

The PULPO repository (Lechtenberg, 2023b) includes demonstrations across case studies from various sectors: optimizing an H_2 production system, an assessment of the energy transition exemplified on the German electricity market, and the deployment of a plastic waste recycling technology for fuel production from an economy-wide perspective. The latter two examples are also described in Supplementary Information S5 and S6, respectively. They illustrate the various functions of PULPO on simple problems, using an unmodified LCI directly obtained from ecoinvent (*electricity problem*) and the same LCI complemented with a user-defined inventory (*plastics recycling problem*).

The following subsections demonstrate the use of PULPO in a more complex case study, optimizing a sector coupling production system, and connecting the electricity sector to the chemical sector via carbon capture and utilization (CCU) processes. The case study employs prospective background databases obtained from premise (Sacchi et al., 2022), to gauge the impact reduction potential from CCU deployment under different scenarios.



(a) Bottom-up inventory construction as done in TCM



(b) Top-down row elimination approach as done in PULPO

FIGURE 2 Strategies to obtain rectangular technosphere matrix for the definition of the optimization problem. In the bottom-up approach, processes from the base life cycle inventory (LCI) are aggregated to be in line with the inventories from other sources such as simulations or literature. Potential links of the processes lost in aggregation and user inventories are omitted. In the top-down approach, rows of equivalent products are added up to form a new row. By doing so, new links between the user inventories and the base LCI are created, and no information is lost in aggregation. Red dotted boxes in the rectangular technosphere matrix indicate product equivalent processes that are subject to optimization. PULPO, Python-based user-defined lifecycle product optimization; TCM, technology choice model.

3.1 | CCU sector coupling case study

Methanol is often claimed as a key enabler molecule (Olah, 2005) for climate change mitigation of the chemical industry (Kätelhön et al., 2019), despite potential burden-shifting to other categories depending on the H_2 source (Galán-Martín et al., 2021). Using PULPO, we perform regionalized life cycle optimization using prospective background databases to find the best conditions and system configurations to produce methanol from CO_2 and H_2 considering environmental criteria. The use of a combined functional unit of methanol and electricity demand reveals and quantifies the interplay between the decarbonization of the chemical industry via electrification and decarbonization of the energy mix based on future scenarios.

Gabrielli et al. (2020) assessed CCU for methanol production, finding that when powered by grid electricity, carbon footprints < 190 kg CO_2eq/kWh would be needed for the CCU-based methanol production to have a lower climate change impact than the coal-based process. Al-Qahtani et al. (2020) also find that renewable wind electricity should be used to further decarbonize the grid instead of supplying CCU methanol

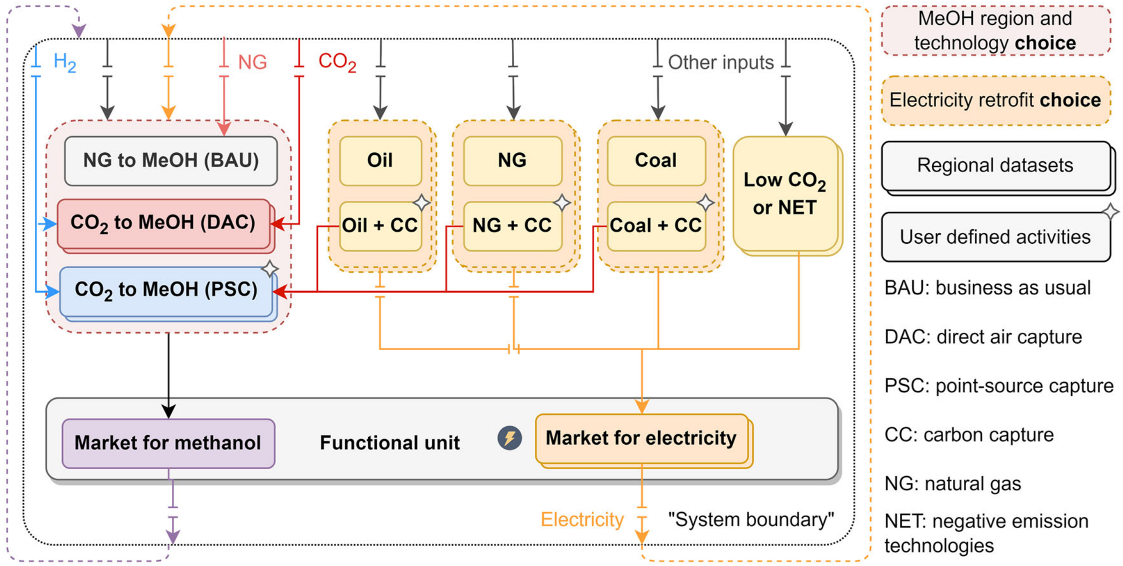


FIGURE 3 Electricity–chemical sector coupling system subject to optimization.

production but argue that this situation is likely to change with progressing decarbonization efforts and technology scaling. These studies overlook the interplay between the foreground and background systems. More precisely, analyzing the large-scale deployment of green methanol in the foreground system is not consistent with the assumption that methanol will still be fully produced through the fossil route in the background system.

The functional unit for this assessment, in line with the economy-wide scope enabled by PULPO, is the production of 100 Mt of methanol, which corresponds to the approximate global demand for methanol in 2023 (Chemanalyst, 2023). Included in the functional unit is the electricity supply projected by the REMIND IAM (Baumstark et al., 2021) for the specific scenarios and years assessed. These data are obtained from the premise (v.1.6.7) scenario report. The methanol demand is introduced in the *f* vector, and the electricity supply is introduced via the bounds on the scaling vector and the slack variables. In this assessment, three scenarios from the REMIND IAM, adhering to the SSP2 ("middle of the road"), have been selected:

- *Base*: worst-case scenario with a temperature increase of **3.5°C** relative to pre-industrial levels.
- *NDC*: current nationally determined contributions (NDC) agreed upon by the parties of the Paris Agreement. The temperature increase is limited to **2.5°C**.
- *PkBudg500*: limits the CO_2 emission peak at 500 Gt; corresponds to a temperature increase of **1.5°C**.

The indicator to be minimized is the GWP. For that purpose, the set of characterization factors provided by "premise_gwp" has been utilized. This function complements the IPCC GWP100a characterization factors with additional H_2 and biogenic CO_2 uptake release flows. Figure 3 illustrates the system boundary, including the functional unit as well as the possible choices in the production system:

Region and technology choice for methanol production: The 12 regions of the IAM have different conditions and capacity limits (electricity production and carbon availability) for abatement of emissions through methanol synthesis from CO_2 and H_2. Within each region, the carbon source is either a point-source capture (PSC), direct air capture (DAC), or natural gas as used in the business-as-usual (BAU) process. Other carbon sources such as biomass, plastic waste, or coal are not within the scope of this assessment.

Retrofit of fossil thermal power plants: IAM scenarios consider the rollout of power plants with carbon capture and storage (CCS). The fraction of plants that is not predicted to implement CCS can potentially be retrofitted with carbon capture for subsequent usage in methanol synthesis. Grid electricity capacity expansion is necessary to support the transition of the chemical sector, which is assumed here to follow the fixed share for the non-fossil production technologies, as projected by the scenario, while the technology choice allows retrofitting of the fossil shares.

The methanol synthesis process from point-source CO_2 is a direct copy of the methanol from DAC CO_2 process as modeled by premise, changing the input of CO_2 from DAC to an auxiliary CO_2 from the PSC market process. This market process is introduced for each region and takes as an input the output of the newly introduced fossil thermal power plant process with retrofitted carbon capture for utilization.

To introduce these power plants with carbon capture activities, all the fossil thermal power plant activities in the LCI database without carbon capture were copied and their inputs were changed using assumptions from Volkart et al. (2013) on CO_2 capture rate, energy penalty, water increase, solvent use, and other emission reductions and increases (see Supplementary Information S7). The captured CO_2 was added together

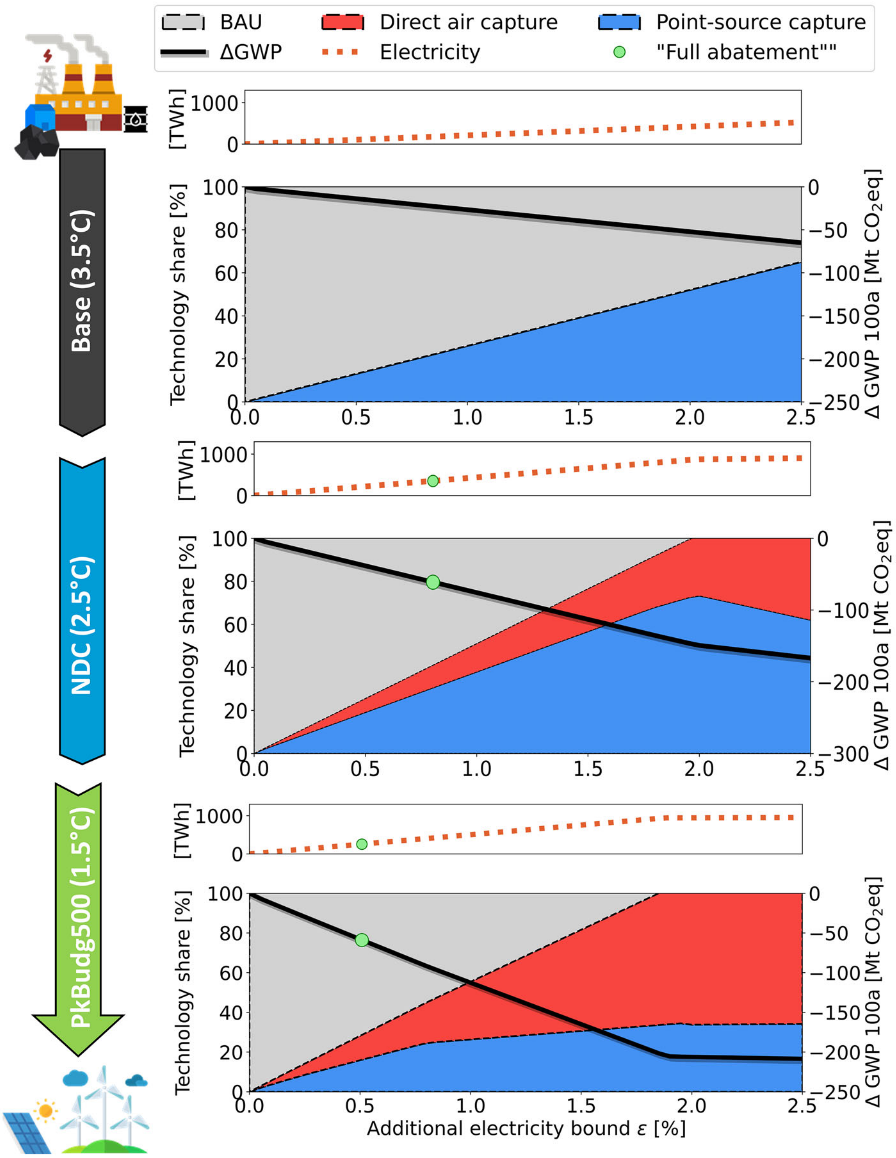


FIGURE 4 Optimized methanol production as a function of additional electricity ε [0.0%, 2.5%] in 2040. Depicted are the global shares of methanol production via business as usual (BAU), direct air capture (DAC), and point-source capture (PSC). The solid black lines represent the change in global warming potential (GWP) [Mt CO_2eq], and the dotted yellow lines show the absolute amount of additional electricity [TWh]. Also indicated are the full abatement situations. Underlying data for this figure are available in Zenodo (Lechtenberg, 2023a).

with the main reference product electricity as an output, making this a multi-functional process. See Table S2 Supplementary Information S7 for an illustration of how the flows are adapted and what the multifunctional process looks like for a hard coal power plant retrofitting inventory. As the auxiliary CO_2 from the PSC market may not be overproduced, every quantity of CO_2 captured in the retrofitted power plants must be utilized in methanol synthesis or otherwise the retrofit may not occur.

The input data for this case study, scripts for the assessments, and post-processing are openly available at Zenodo (Lechtenberg, 2023a).

3.2 | Global production mix for methanol

Methanol production via CO_2 and H_2 routes relies on large amounts of electricity, and the future production system will depend on the availability of low-carbon electricity. Figure 4 illustrates the optimal technology share (BAU, DAC, PSC) for the three selected scenarios (Base, NDC, and PkBudg500) in 2040 as a function of additional electricity production capacity available. The reference for “additional electricity” and the GWP reduction “ΔGWP” is the non-optimized system (i.e., electricity is supplied from the unaltered markets and methanol via BAU, without the option of CCU) in the corresponding scenario and year, fulfilling the same final demand. When CCU is available as a choice and implemented, the total GWP reduces with respect to the reference situation. This reduction is at the expense of additional electricity production capacity installed, necessary for CCU.

It can be seen how abatement (in terms of ΔGWP [kg CO_2eq]) takes place as a function of total additional electricity capacities installed (in TWh). The year 2040 has been selected because the difference in decarbonization progression between the scenarios is large. The base scenario has a low rollout of low-carbon technologies, NDC has a more advanced rollout, and the PkBudg500 scenario has already approached its final state to comply with the specified climate goals (see Figure S7 in Supplementary Information S8).

The CCU optimization problem is solved, activating the choices for retrofitting power plants and synthesizing methanol from CO_2 and H_2. For the capacity constraints, an electricity-bound parameter ε is introduced. It is defined as an upper bound according to Equation (5):

$$s_j^{\text{high}} = (1+\varepsilon)\cdot s_j^{\text{low}} \qquad \forall j \in \{\text{name } (j) = \text{market for electricity, high voltage}\} \tag{5}$$

Here, s_j^{low} corresponds to the electricity supply projected by the IAM, for all processes j that are electricity markets (high voltage) in each region. The constrained problem was solved repeatedly for 51 linearly spaced values of ε between 0.0% and 2.5%. We may argue that this is a marginal increase over 15 years. Although the problem could be enriched with additional infrastructure, indicators, or environmental flow constraints, these elements are not considered here.

The computational complexity of the linear problems depends on the scenario, which affects the number of power plants and choices involved. For the PkBudg500 scenario in 2040, there are 27,599 processes in the LCI, resulting in 55,493 variables when considering impact and slack variables. There are 184 choices for power plant retrofit processes and 26 for methanol production processes. Additionally, there are 27,391 equality constraints for the functional unit and impact calculations, along with inequality constraints on the scaling vector and slack variables, totaling 111,406 constraints. The problem was solved on a Windows 10 computer with an Intel Core™ i7-12700K processor using the cplex 37.1.0 solver in less than 3 s.

The results are shown in Figure 4. It can be seen that even under a moderate decarbonization scenario, the use of additional electricity to produce PSC or DAC-based methanol would reduce the overall GWP. This means that the potential reduction of replacing BAU methanol compensates for the impact incurred from the production of additional electricity. The more stringent the decarbonization scenario, the more effective the decarbonization of the chemical industry via abatement, which is indicated by the steeper ΔGWP curve, from top to bottom scenarios.

Moreover, DAC-based methanol plays a key role in the NDC and PkBudg500 scenarios due to the limited availability of carbon sources from fossil thermal power plants without CCS. This can be interpreted as an imperative shift toward carbon circularity via air capture of CO_2. It should be acknowledged though that the scope of this assessment does not include other point sources of CO_2 such as cement kilns or the possibility of using already captured CO_2 destined for storage in utilization instead. Likewise, other potential renewable carbon sources for green methanol like plastic waste or biomass are not considered. Additionally, specifying a global demand for methanol does not account for the distribution from production sites to the actual locations of demand. This omission should be considered when interpreting the results.

3.3 | Regional methanol production for full abatement

We define "full abatement" as the total compensation of carbon emissions (GWP reduction) otherwise incurred by the BAU process. This target depends on the scenario: Figure 4 illustrates this full abatement situation for the base, NDC, and PkBudg500 scenarios in 2040 as the green dots. See Supplementary Information S10.1 for a detailed breakdown and description of the full abatement case of these situations.

The results are not only detailed in terms of technology but also regional choices. Figure 5 shows the geospatial distribution of the optimized methanol production systems reaching full abatement for the PkBudg500 (1.5°C) scenario in the years 2030, 2040, and 2050. Illustrated are the absolute production volumes in each region and the qualitative share between PSC and DAC-based routes indicated through shades of red and blue. In the lower-left corner, the remaining production via BAU is stated. There are 12 regions in the REMIND IAM. Table S3 in Supplementary Information S9 shows the name of each region.

With progressing decarbonization, the importance of DAC clearly increases. This is conditioned by the previously mentioned effect of diminishing carbon sources in the electricity sector. However, the degree of transition is different from region to region. For instance, in Sub-Saharan Africa (SSA), the production volumes are 1.1 Mt via PSC (2030), 1.3 Mt via mixed DAC/PSC (2040), and 2.1 Mt via DAC (2050). On the other hand, in Russia (RUS), the production volumes are 1.9 Mt via PSC in 2030 and 1.0 Mt via mostly mixed DAC/PSC in 2040 and 2050. The electricity market of SSA evolves such that DAC becomes the technology that reduces the GWP most efficiently. In Russia, there is a large remaining share of fossil thermal power plants that favor the implementation of PSC methanol. This illustration further underlines the importance of shifting toward fully circular carbon, in this scope via DAC, within a decarbonizing world.

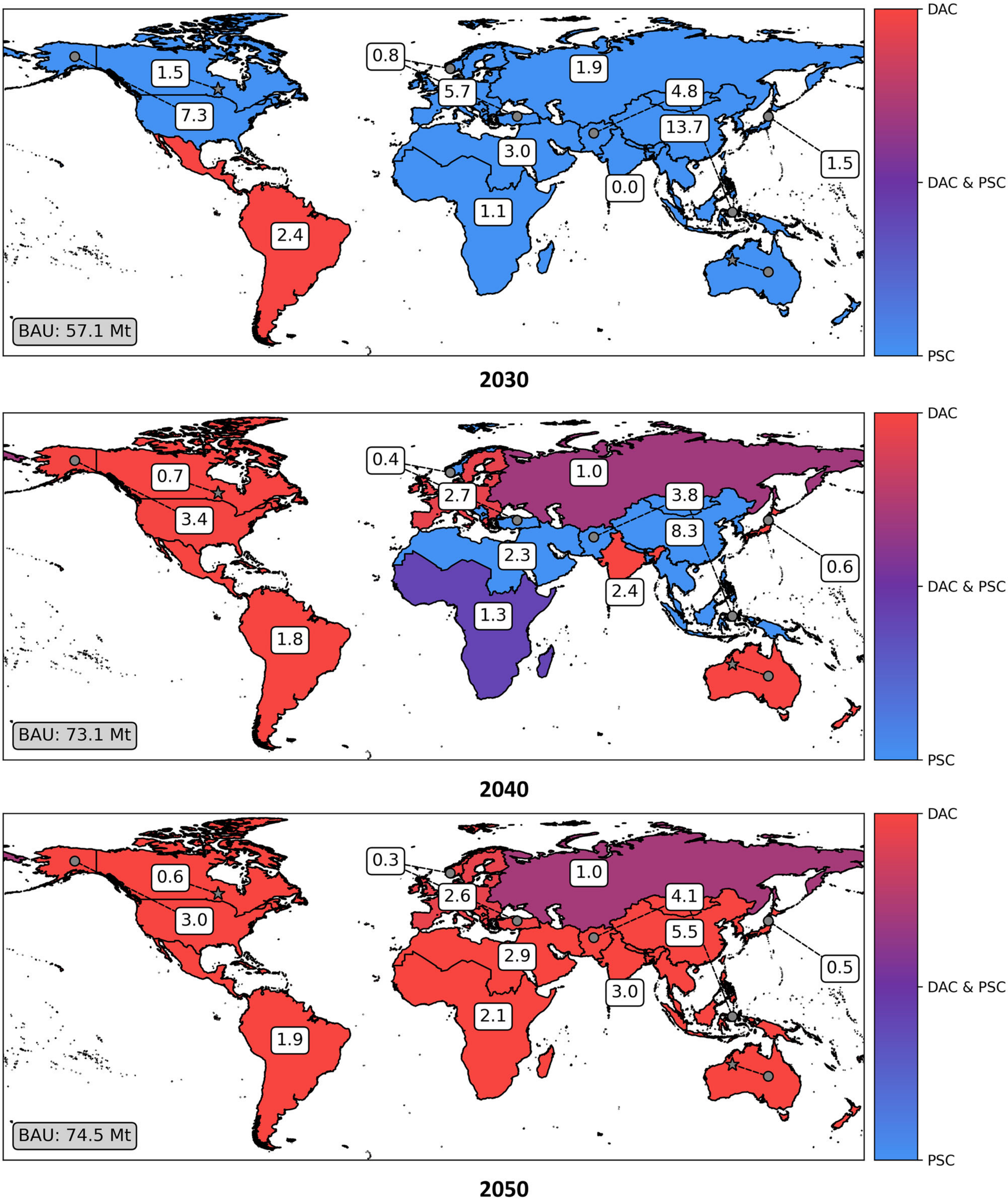


FIGURE 5 Geospatial distribution of optimized full abatement methanol production systems according to PkBudg500 (1.5°C) scenario in 2030, 2040, and 2050. Underlying data for this figure are available in Zenodo (Lechtenberg, 2023a). BAU, business as usual; DAC, direct air capture; PSC, point-source capture.

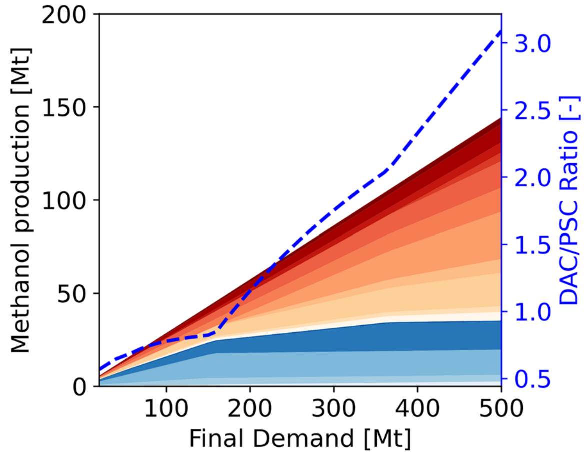


FIGURE 6 Final demand variation of methanol for the full abatement situation in the 2040 PkBudg500 (1.5°C) scenario. Direct air capture (DAC) production for different regions is indicated in shades of red, point-source capture (PSC) production in shades of blue, and business-as-usual (BAU) production is omitted in the representation. The ratio of DAC to PSC is illustrated via the blue dotted line. Underlying data for this figure are available in Zenodo (Lechtenberg, 2023a).

3.4 | Influence of methanol demand

Up to this point, a final methanol demand of 100 Mt has been assumed, which is approximately the current global demand. However, the demand for methanol is likely to increase in all sectors (Bhosale & Sanka, 2022), especially when taking into account its potential for the basis of a methanol economy (Simon Araya et al., 2020), meaning that methanol plays a fundamental role both as energy vector as well as hydrocarbon source for the chemical industry. The assessment shown in Figure 5 can be easily repeated by adjusting the methanol part of the functional unit.

Figure 6 shows the results for values ranging between 20 and 500 Mt. It is clear that the importance of DAC increases with increasing chemical demand. This is mainly due to the carbon availability limitation mentioned before.

4 | CONCLUSION AND FUTURE WORK

This paper has introduced the PULPO framework for LCO. From a methodological point of view, the framework for the first time allows the specification and optimization of choices in the background system using complete LCI databases as the backbone, which enables the comprehensive assessment of technologies and pathways from an economy-wide perspective, taking into account all possible feedback loops. This has been exemplified in a case study focusing on the sector coupling of the energy and chemical industry, a case which, due to its complex interactions across the whole supply chain extending into the background, would have been impractical to be assessed otherwise.

From an implementation point of view, the framework is complemented with a convenient open-source Python package that allows for fast uptake of the approach within the targeted LCA and PSE communities with little prior expertise required.

It has been shown that the framework can provide comprehensive analyses, particularly in assessing environmental impacts and identifying optimal solutions across multiple scenarios, scales, and impact categories, as evidenced by our case studies. It is particularly useful for conducting LCA and optimization concurrently, enabling life cycle optimization of product systems where the foreground and background systems are varied together, according to environmental criteria and capacity, indicator, or environmental flow constraints. This leads to insightful analyses where a plethora of scenarios can be screened automatically using optimization algorithms without the need to define them manually, including changes in the background system that are often assumed fixed in standard LCAs and LCOs.

PULPO was applied to optimize future methanol supply chains under different climate policy scenarios. The findings of these studies emphasize the importance of pursuing carbon circularity through DAC and, very likely, using other sources of renewable carbon omitted in this analysis, as decarbonization efforts continue to intensify worldwide. Additionally, the results highlight the strong coupling between the electricity and chemical sectors, revealing an asymmetrical but interdependent relationship between these two areas.

The usefulness of our framework critically hinges on data quality. While databases such as ecoinvent are intended to be a good representation of current production systems, they are not exempt from caveats as pointed out for instance by Bicalho et al. (2017). Moreover, the presented case study relies not only on the commercial ecoinvent LCI but also on prospective IAM-based derivatives from an open-source application (premise). This adds several, potentially conflicting, assumptions and a fair amount of uncertainty to the assessment. However, the obtained results are coherent with the assumptions made. Moreover, the insights obtained can be explained from our previous knowledge of this type of system and an in-depth analysis of the results, while no major data quality issues were identified. Another limitation of the approach follows from the top-down nature of defining the problem. Since choices are defined on an equivalent product basis, the user should check and restrict potentially conflicting substitutions that may occur.

One potential future research direction would be to utilize the lognormal distributions used to model the uncertain LCI data following the pedigree matrix (Frischknecht et al., 2005) to formulate probabilistic constraints under a robust optimization framework. The goal would then be to minimize the expected value of the impact while imposing a bound on the probability of exceeding a certain target value, similar to previous demonstrations dealing with the design and planning of supply chains (Guillén-Gosálbez & Grossmann, 2009). The integration of economic or social data, for example, using PSILCA (Maister et al., 2020), could further enhance the capabilities of LCI databases. It could lead to more holistic and impactful assessments, providing a more comprehensive picture of a product's environmental impact throughout its entire life cycle. To further support this comprehensive picture, improvements to the exploration of the obtained results via visualization and filtering techniques should be considered. Being a modular open-source platform, PULPO is expected to integrate several optional features, including functions already available in adjacent tools such as multi-objective and multi-period optimization and novel customized functions such as non-linear objectives and constraints.

From a broader perspective, this work is intended to build bridges between the industrial ecology and process systems engineering communities. Through cross-fertilization of ideas, we will perform more insightful analyses to make better decisions in the quest for sustainability.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are openly available in Zenodo at https://doi.org/10.5281/zenodo.12790643, reference number 12790643.

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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