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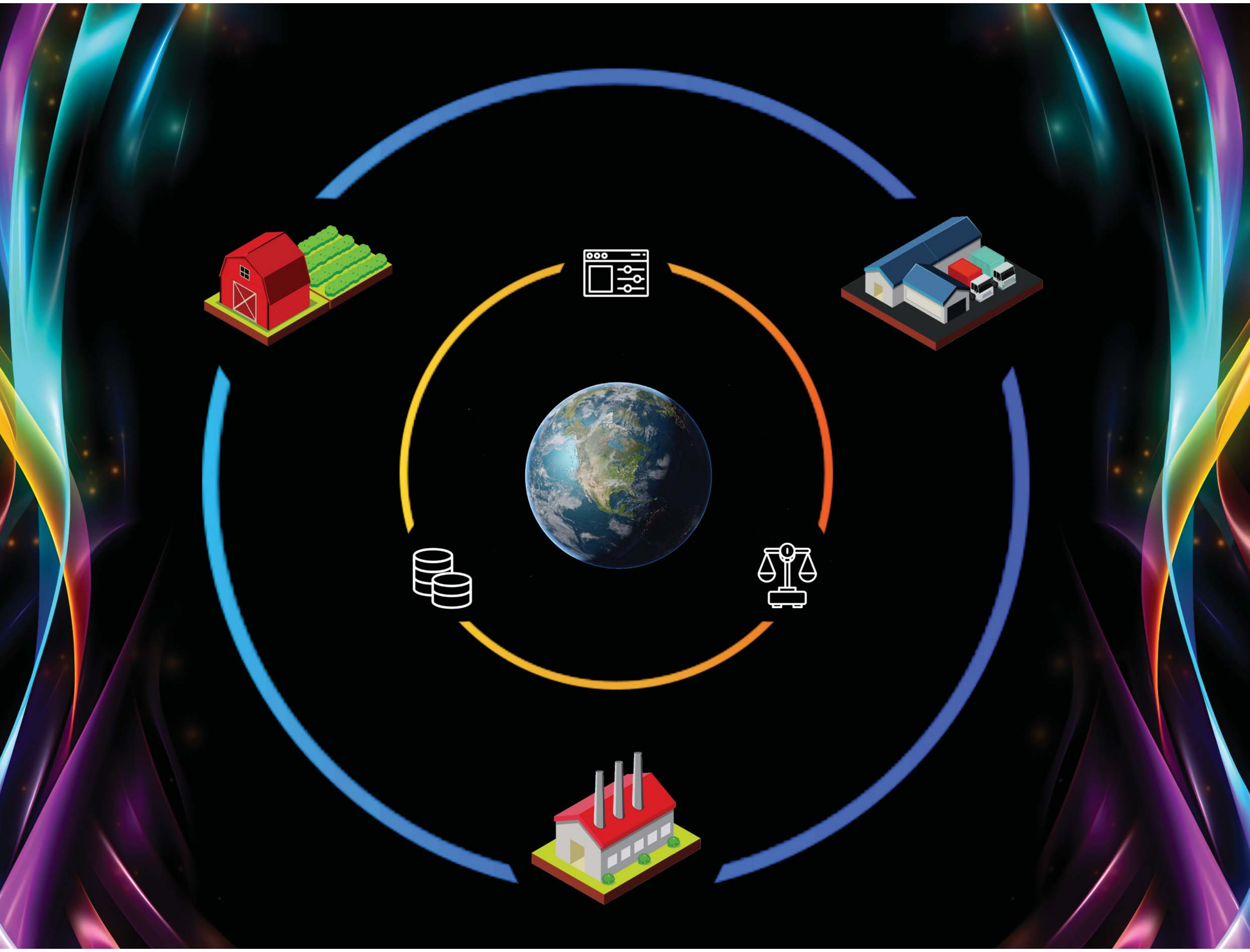

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Life cycle optimisation tool development for process systems and centralised supply chain design†

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Historically, optimisation processes for supply chains have primarily focused on maximising economic objectives. However, with the challenges posed by climate change, there has been a shift towards integrating environmental considerations into optimisation processes alongside economic criteria, which can be facilitated by life cycle assessment. This approach enables supply chain managers to move beyond solely analysing emissions from individual plants, instead considering all life cycle stages. Yet, despite the advancements made in incorporating environmental considerations, the challenge lies in identifying the most effective improvement strategies and selecting optimal alternatives within decision environments characterised by multiple and often conflicting objectives. Real-life scenarios frequently demand simultaneous economic and environmental criteria considerations to ensure products' sustainability over their entire life cycle. Striking a delicate balance between these divergent objectives requires careful evaluation, innovative solutions, and robust decision-making processes. One of the solutions is combining multi-objective optimisation with life cycle assessment because of its ability to balance environmental and economic performance. By leveraging this approach, decision-makers can navigate the trade-offs between these two crucial aspects, empowering them to select the most appropriate solution that aligns with their specific requirements, constraints, and objectives. A decision-aid toolkit has been developed in this paper and validated using a real-life case study focused on electricity generation in the UK. This practical application showcases the methodology's effectiveness and provides tangible evidence of its potential to drive improvements in the real world.

Sustainability spotlight

To address sustainability development goals (SDG), we need to consider conflicting environmental objectives. In the past decades, efforts have been placed to develop life cycle assessment (LCA) methods and databases representing the averaged technologies and quantitative approaches to characterise the environmental footprints. However, LCA only enables retrospective data analysis and evaluation functions but does not inform the real-world decision-making, which is often based on site-specific data and consists of multiple solutions within the given decision spaces. Under this context, we developed a new modelling toolbox underpinned by mathematical optimisation and LCA to harness state-of-the-art LCA database advances and enable users to derive optimal solutions considering multiple sustainability criteria. The energy systems optimisation study demonstrated the model applicability and functionality.

Introduction

Background

The current state of the environment on Earth paints a concerning picture. The temperature has already increased by around 1.1 °C compared to the late 1800s, which makes the current temperature the highest it has been in the last 100 000 years.[1] To avoid the severe impacts and maintain a habitable planet, it is widely recognised that limiting temperature rise to less than 1.5 °C is crucial.[2] The Paris Agreement 2015 marked a significant step in tackling climate change. Countries worldwide pledged to adopt nonbinding national targets to reduce greenhouse gas emissions.[3] More recently, the 2021 Conference of the Parties placed a renewed emphasis on staying on track to meet these targets. A significant development arising from the 2021 Conference of the Parties was the widespread adoption of net zero by 2050 as a target.[4]

Recognising the urgency of the climate crisis, the UK government has made ambitious promises to curtail emissions. They have set targets to slash emissions by 68% by the end of the decade, 78% by 2035, and 80% by 2050, all compared to 1990.[5] To achieve these goals, the UK government has

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implemented a cap on total greenhouse emissions every five years, further underlining their dedication to mitigating climate change.[6] The commitment to limit global warming and the adoption of net zero targets reflects the growing recognition of the need for urgent and comprehensive measures. Stakeholders across various sectors must embrace a systematic approach, consider the entire value chains, and work collaboratively to achieve these ambitious goals and ensure a sustainable and resilient future for next generations.

It is of great importance to accurately define net zero in this context. Fundamentally, net zero means that the rate of emissions and the rate of removal from the atmosphere are equal, such that the accumulation of greenhouse gases is zero. Defining the scope of net zero targets is essential to clarify what emissions are accounted for. A company's greenhouse gas emissions (GHG) include its direct emissions (scope 1) and indirect emissions from the production and transmission of energy (scope 2) as well as indirect emissions from up- and downstream activities along the value chain (scope 3).[7] The scope 3 represents more than 80% of emissions for most industries.[8] To this end, it is crucial to adopt a system-thinking approach and set net-zero targets across three scopes to reduce emissions across the entire value chain. One method that has gained significant traction as a well-established approach to assessing the environmental effects of entire systems is life cycle assessment, which takes a holistic view of the system and moves beyond assessing system viability solely based on financial budgets by incorporating environmental impacts.

Globally, governments and companies have made their net zero commitments, and the focus has shifted towards devising strategies to achieve these goals, taking immediate action, and ensuring transparent reporting through regular progress updates. Moving towards net-zero emissions is a critical goal for industries worldwide, but it comes with a set of challenges. First, the initial capital investment required for transitioning to net-zero operations can be substantial. Industries may struggle with finding the financial resources to make these changes, especially for small and medium enterprises. Second, achieving net-zero emissions often involves working with suppliers and partners to ensure that the entire value chain is sustainable. This can be challenging due to variations in the sustainability practices of different stakeholders. Multiple Criteria Decision-Making (MCDM) can play a crucial role in navigating these challenges. MCDM is a systematic approach that involves evaluating and comparing various alternatives based on multiple criteria or objectives. MCDM helps industries consider a range of criteria, including environmental impact, cost, feasibility, and social acceptance. This enables a more balanced decision-making process. MCDM also allows industries to perform scenario analysis and sensitivity testing to assess how changes in different criteria affect the overall decision. This helps in identifying robust solutions. By utilising MCDM, industries can systematically evaluate and prioritize actions to move towards net-zero emissions in a way that aligns with their specific goals, constraints, and stakeholder interests.

Transitioning to net zero systems necessitates decision-making processes that balance environmental considerations with traditionally economically focused practices. A potential solution to this challenge lies in leveraging mathematical optimisation techniques to determine optimal strategies for achieving net zero while adhering to economic constraints. The project employs different optimisation methods to navigate the vast solution space and uncover the optimal solutions within a centralised supply chain context. Firstly, a mixed integer linear programming model is developed to formulate the optimisation problem. Secondly, genetic algorithms, renowned for their efficacy in solving complex optimisation problems, are applied to yield optimal or near-optimal solutions that align with the identified objectives. End-users can select from various pre-existing processes through a comprehensive toolkit, configure their supply chain system parameters, and obtain valuable insights about emissions and economic advantages.

It is acknowledged in the research that often supply chains employ decentralised decision-making, allowing each participant to autonomously determine their course of action. This introduces a multi-player dimension to supply chain design, presenting research challenges in both modelling and computational aspects.

Life cycle assessment

Life cycle assessment (LCA) quantifies the environmental impacts associated with all stages of a product, service, or process from cradle-to-grave. LCA offers a systems approach and provides holistic insights on environmental scores to inform decision making. LCA comprises four stages: goal and scope definition, life cycle inventory analysis, life cycle impact assessment (LCIA), and interpretation.[10] The process of defining the purpose and breadth of a study involves the establishment of its objectives, boundaries, and intended applications. Life cycle inventory analysis includes data collection on each stage's various inputs and outputs. LCIA associates inventory with environmental categories and category indicators to quantify the environmental footprint. Finally, the interpretation stage includes scrutinising and communicating the findings while considering the constraints and uncertainty of the evaluation.

Direct measurements, expert opinions, evaluations based on empirical observations, and computer simulations are some of the various methods that can be used to construct life cycle inventories.[11] Among them, the estimation method has seen widespread use, as seen by the Eco-invent inventories for infrastructure,[12] energy usage and CO_2 estimation of organic chemicals.[13] By utilising these methods, datasets that represent the typical processes for geographical areas or industries have been generated, which are typically used to supplement the site-specific data that is utilised in LCA models. The datasets that are accessible to the public might be categorised as either national/regional datasets, or industry datasets. The former is created by combining regional datasets to show national or international inventories for products or services; examples of this include the NREL US LCI databases that were created in 2004.[43] Industrial associations are typically responsible for the development of industrial datasets, which are designed to generally represent industry-average processes or products.

Some examples of industrial datasets include the datasets for plastic products that were generated by Plastics Europe,[44] and the EU corrugated board database that was developed by FEFCO.[45] Some of the databases that were mentioned before having been incorporated into commercially accessible software for LCA modelling. Examples of such software include SimaPro, GaBi, and openLCA, all of which feature a variety of datasets at global scale, which cover a wide range of industries and geographies.

LCIA methodologies can be categorised as midpoint and endpoint-oriented approaches which are also termed as 'problem-oriented' and 'damage approach' respectively. The former is chosen along with environmental mechanisms between the LCI results and endpoints whereas the latter is defined at the level of protection are. A range of LCIA methodologies have been developed and introduced as method library embedded in commercial LCA software. Generally, three input-related environmental categories are considered in LCA *i.e.*, resource depletion and land and water use; other categories are output-related *e.g.*, global warming potential, acidification, eutrophication. ReCiPe is one of the widely accepted approaches to impact evaluation. The first version of it was created in 2008, while the most recent one was released in 2016. ReCiPe evaluates numerous impact categories at the midpoint level, and at the endpoint level, it evaluates the three areas of human health protection, ecosystem quality protection, and natural resource.[15]

Optimisation method

The classification of optimisation algorithms is divided into two categories: mathematical programming methods[16] and heuristics solution search algorithms.[17] Classical techniques, such as those based on gradient or linear algebra, utilise mathematical properties to explore the search space and achieve convergence towards the best solution. They may encounter difficulties when dealing with problems exhibiting high-dimensional search spaces and non-linear objective functions, frequently seen in practical engineering scenarios. In such instances, conventional algorithms may prove inadequate in yielding desirable outcomes or inapplicable due to their dependence on certain assumptions or simplifications. Modern optimisation algorithms are developed to address the limitations of classical optimisation algorithms, specifically tailored to overcome the challenges of complex optimisation problems. These algorithms often draw inspiration from biological processes and natural phenomena. They emulate natural principles, such as natural selection, genetic variation, or collective behaviour, to navigate the search space efficiently and discover near optimal or globally optimal solutions. Some examples of heuristics solution search algorithms include genetic algorithm,[18] particle swarm optimisation algorithm,[19] ant colony optimisation algorithm[20] and coral reefs optimisation algorithm.[21] Among those, genetic algorithm is the most widely used one.

Multi-objective optimisation poses a greater complexity than single-objective optimisation because several objective functions must be considered simultaneously. There are two primary ways to deal with the problem. *A priori* method involve assigning weights or priorities to objectives before analysing the data, a typical example is the weighted sum method, where each objective function is multiplied by a weight and summed to form one objective. The weights are assigned based on the importance of objectives. Alternatively, *a posteriori* method involves analysing the data first and making decisions based on the observed outcomes or satisfying defined constraints. A critical concept in this context is Pareto-optimal solutions, which refer to solutions not dominated by other solutions. One method can be used to find Pareto front is the epsilon-constraint method. In this approach, one objective function remains unchanged while the others are constrained within specific values. Careful selection of the epsilon value is crucial to ensure successful implementations.

Real-world applications frequently present constrained multi-objective optimisation problems, and evolutionary algorithms are commonly used to obtain a group of near-optimal feasible solutions. A non-dominated ranking is utilised when determining the order of the solutions in domination-based constrained multi objective evolutionary algorithms. Methods such as the adaptive trade-off model,[22] infeasibility-driven evolutionary algorithm,[23] NSGA-II with constrained dominance principle,[24] and self-adaptive penalty[25] are some representative examples. On the other hand, a multi-objective optimisation problem is broken down into several single objective optimisation subproblems in the decomposition-based algorithms. Methods such as CMOEA/D,[26] MOEA/D-CDP,[27] MOEA/D-SR,[27] and MOEA/D-IEpsilon[28] are a few examples.

Life cycle optimisation

As above-mentioned, LCA offers a technique to evaluate the environmental burdens of products. In past decades, efforts have been placed to develop LCA databases representing the averaged technologies and quantitative methods to characterise the ecological implications. However, LCA only enables retrospective data analysis and evaluation functions but does not inform the real-world design problems, which are often based on site-specific data and consist of a few solutions. Real-world decision-making involves identifying the optimal or near-optimal solutions within the given decision spaces. A modelling approach underpinned by mathematical optimisation and LCA offers a promising way to support such multi-criteria decision-making.

Previous research efforts have been placed to couple LCA and optimisation. Some studies focused on environmental objectives, *e.g.*, optimisation for biodiesel production using waste oil while minimising several environmental impacts of the process.[29] Whereas, other research not only considered ecological objectives but also economic objectives. For example, optimising a nitric acid plant with the goals of financial returns and environmental index function,[30] optimising an mining and processing system to minimise impacts from the system, while maximising production and lowering the costs,[31] optimisation for building retrofitting with consideration of economy, energy and environment criteria,[32] optimisation for hydrogen supply chain design with objectives of cost and global warming potential using epsilon-constrain method,[33] optimising the design of biofuel supply chains with objectives of the cost, the greenhouse gas emissions, and the number local jobs,[34] and optimising the design of CHP-based microgrids with the global warming potential and the acidification potential serving as the objectives.[35]

Despite the previous published work, research gap remains open on LCA optimisation tool development, which harnesses state-of-the-art LCA database and offers potential for end-users to derive optimal solutions considering site-specific value chain data and multiple sustainability criteria. To fill this gap, our research not only proposes a determinacy LCA optimisation model, but also develops a software that uses modern graphical user interface toolkit. These models effectively capture and mathematically represent the transformations and production activities of complex supply chain systems by applying the principles of process systems engineering.[9] The work focuses on proof-of-concept for the software toolbox and aims to verify the feasibility, practicality, and potential of coupling LCA and multi-objective optimisation. The model proposed in the study considers a wide variety of goals, ranging from maximising profits to minimising negative effects on the environment as determined by LCA techniques. To navigate the high-dimension solution space and discover the outcomes that are the most optimal within the context of a supply chain, this work uses a variety of different optimisation methods. Using the toolkit end-users could choose from a variety of pre-existing processes, set the parameters of their supply chain systems, and gain useful information regarding emissions and the economic benefits.

Methodology

Optimisation model development

A linear programming model has been developed building upon LCA and optimisation theory. The constraints of the optimisation model and the objective functions for supply chains are shown below. The sets and indices, variables, and parameters are listed in Table 1.

The resource used by a particular production process during the considered time span for a given location is calculated by eqn (1).

$$R_{r,p,l} = \sum_{y \in \mathrm{SY}} \frac{X_{c,l,y}}{D_p} R_{r,p,l,y} \tag{1}$$

Similarly, the resource consumed by a transmission process is shown in eqn (2)

$$R_{r,t,l} = \sum_{y \in \mathrm{SY}} \frac{X_{c,l,y}}{D_{\mathrm{out},t}} R_{r,t,l,y} \tag{2}$$

A finite amount of a resource is available for a supply chain. In eqn (3), the maximum amount of each resource that can be utilised is specified.

$$R_r^{\lim} \geq \sum_{l \in \mathrm{SL}} \sum_{p \in \mathrm{SP}} R_{r,p,l} + \sum_{l \in \mathrm{SL}} \sum_{t \in \mathrm{ST}} R_{r,t,l} \tag{3}$$

Eqn (4) represents the emission produced by a production process during a certain time period.

$$E_{r,p,l} = \sum_{y \in \mathrm{SY}} \frac{X_{c,l,y}}{D_p} E_{e,p,l,y} \tag{4}$$

The emissions related to each transmission process is represented in eqn (5).

$$E_{r,t,l} = \sum_{y \in \mathrm{SY}} \frac{X_{c,l,y}}{D_{\mathrm{out},t}} E_{e,t,l,y} \tag{5}$$

In addition, upper limitations are placed to bound the total amount of emissions, as shown by eqn (6).

$$E_e^{\lim} \geq \sum_{l \in \mathrm{SL}} \sum_{p \in \mathrm{SP}} E_{e,p,l} + \sum_{l \in \mathrm{SL}} \sum_{t \in \mathrm{ST}} E_{e,t,l} \tag{6}$$

To ensure that the total amount of the product produced by the supply chain is greater than or equal to the demand, eqn (7) is applied.

$$D^{\lim} \leq \sum_{l \in \mathrm{SL}} \sum_{y \in \mathrm{SY}} \sum_{c \in \mathrm{SC}} X_{c,l,y} - \sum_{l \in \mathrm{SL}} \sum_{y \in \mathrm{SY}} \sum_{t \in \mathrm{ST}} \frac{X_{c,l,y}}{D_{\mathrm{out},t}} (D_{\mathrm{in},t} - D_{\mathrm{out},t}) \tag{7}$$

The output amount of the product is equal to the input amount times the loss rate of a transmission process, as given in eqn (8).

$$D_{\mathrm{out},t} = D_{\mathrm{in},t} L_t \tag{8}$$

Eqn (9) shows that the amount produced by each production process should be equal to the input of each transmission process.

$$\sum_{l \in \mathrm{SL}} \sum_{y \in \mathrm{SY}} \sum_{c \in \mathrm{SC}} X_{c,l,y} = \sum_{l \in \mathrm{SL}} \sum_{y \in \mathrm{SY}} \sum_{t \in \mathrm{ST}} \frac{X_{c,l,y}}{D_{\mathrm{out},t}} D_{\mathrm{in},t} \tag{9}$$

The transportation cost of the supply chain is calculated by eqn (10).

$$T^{\mathrm{total}} = \sum_{y \in \mathrm{SY}} \sum_{l \in \mathrm{SL}} \sum_{p \in \mathrm{SP}} \frac{X_{c,l,y}}{D_p} H_{p,y} T_p + \sum_{y \in \mathrm{SY}} \sum_{l \in \mathrm{SL}} \sum_{t \in \mathrm{ST}} \frac{X_{c,l,y}}{D_{\mathrm{out},t}} H_{t,y} G_t \tag{10}$$

The profit for each production process is given in eqn (11).

$$J_p^{\mathrm{total}} = \sum_{y \in \mathrm{SY}} \sum_{l \in \mathrm{SL}} \sum_{p \in \mathrm{SP}} \frac{X_{c,l,y}}{D_p} (B_{p,y} - C_{p,y}) + \sum_{y \in \mathrm{SY}} \sum_{p \in \mathrm{SP}} G_{p,y} \tag{11}$$

Similarly, the profit for each transmission process is given in eqn (12).

Table 1 Sets and indices, variables, and parameters

	Definitions	Unit
Sets and indices		
$p \in$ SP	Subset of production processes	
$t \in$ ST	Subset of transmission processes	
$f \in$ SF	Subset of flows	
$c \in$ SC	Subset of processes	
$r \in$ SR	Subset of resource flows	
$e \in$ SE	Subset of emission flows	
$l \in$ SL	Subset of locations	
$y \in$ SY	Subset of years	
KPI	Set of key performance indicator	
Variables		
$E_{\text{kpi}}^{\text{total}}$	Total impact on the environment caused by emission on a given KPI	(Amount)
A^{total}	Revenue of the entire supply chain	(£)
J_p^{total}	Profit for each production process	(£)
J_t^{total}	Profit for each transmission process	(£)
T^{total}	Transportation cost of the entire supply chain	(£)
$X_{c,l,y}$	Continuous variable representing amount of product of each process	(Number)
Parameters		
D_p	Production capacity per process	(Amount)
$R_{r,p,l,y}$	Resource inventory of each production process	(Amount)
$R_{r,p,l}$	Resource used by a production process during a certain period	(Amount)
$D_{\text{out},t}$	Output amount of product for each transmission process	(Amount)
$R_{r,t,l,y}$	Resource inventory of each transmission process	(Amount)
$R_{r,t,l}$	Resource used by a transmission process during a certain period	(Amount)
E_e^{lim}	Upper bound of emission	(Amount)
$E_{e,p,l,y}$	Emission inventory of each production process	(Amount)
$E_{r,p,l}$	Emission produced by a production process during a certain period	(Amount)
$E_{e,t,l,y}$	Emission inventory of each transmission process	(Amount)
$E_{r,t,l}$	Emission produced by a transmission process during a certain period	(Amount)
D^{lim}	Demand for the product	(Amount)
$D_{\text{in},t}$	Input amount of product for each transmission process	(Amount)
$G_{p,y}$	Government subsidy for each process	(£)
L_t	Loss rate for each transmission process	(%)
R_r^{lim}	Resource availability limit	(Amount)
$B_{p,y}$	Unitary revenue of each production process	(£)
$C_{p,y}$	Unitary production cost of each production process	(£)
$H_{p,y}$	Unitary transportation cost of each production process	(£)
T_p	Transportation distance of each production process	(km)
$B_{t,y}$	Unitary revenue of each transmission process	(£)
$C_{t,y}$	Unitary transmission cost of each transmission process	(£)
$H_{t,y}$	Unitary transportation cost of each transmission process	(£)
T_t	Transportation distance of each transmission process	(km)
$F_{f,\text{kpi}}$	Impact factor for each flow	(Impact eq./unit emission)

$$J_t^{\text{total}} = \sum_{y\in \text{SY}}\sum_{l\in \text{SL}}\sum_{t\in \text{ST}}\frac{X_{c,l,y}}{D_{\text{out},t}}\left(B_{t,y} - C_{t,y}\right) \tag{12}$$

The overall profit of the supply line is calculated by eqn (13).

$$A^{\text{total}} = J_p^{\text{total}} + J_t^{\text{total}} - T^{\text{total}} \tag{13}$$

The effect of emissions on the environment is calculated by eqn (14).

$$E_{\text{kpi}}^{\text{total}} = \sum_{e\in \text{SE}}\sum_{l\in \text{SL}}\sum_{p\in \text{SP}}E_{e,p,l}F_{e,kpi} + \sum_{e\in \text{SE}}\sum_{l\in \text{SL}}\sum_{p\in \text{SP}}E_{e,t,l}F_{e,\text{kpi}} \tag{14}$$

This optimisation problem formulation involves aligning the different spatial and temporal dimensions within a supply chain, a crucial aspect for uncovering its most efficient design and operations. Users can set the location, namely, longitude and latitude, of each process and take geographical relationships between different processes within a supply chain into consideration. By changing the revenue according to market demand and subsidy according to government policies and setting the corresponding profit for each year in the toolbox, users can explore different time scales, which enables long-term planning and strategy development.

In single objective optimisation, solver GLPK is used, while NSGA-II is to solve multi-objective optimisation problem.

In the model, both environmental and economic criteria are taken into consideration. There are two methods used in this project to deal with the multi-objective nature of the optimisation problem. First, the weighted sum method is applied to convert the two objectives into one with the meaning of economic value and the unit of pounds. In this case, GLPK is used as the solver. Other than the weighted sum method, another way is using NSGA-II-CDP.

In a genetic algorithm, a population of candidate solutions (individuals or chromosomes) is evolved over multiple generations to find the best solution or a near-optimal solution. The steps of a genetic algorithm are as follows: (1) *Initialisation*: a few individuals are created, each with its own set of characteristics or chromosomes. (2) *Fitness evaluation*: individuals in the population are evaluated using a fitness function that quantifies its quality or suitability as a solution to the problem. (3) *Selection*: populations with higher fitness scores are selected for reproduction. (4) *Crossover*: the selected individuals undergo crossover or recombination, which involves exchanging genetic material (genes or parts of the chromosome) between them. This process produces new offspring with characteristics inherited from their parents. (5) *Mutation*: occasionally, a random mutation is applied to the offspring's chromosomes, introducing small random changes to their characteristics. (6) *Replacement*: the new offspring and some individuals from the previous generation replace the existing population. The replacement can be done based on fitness values or other selection strategies. (7) *Termination*: the algorithm continues evolving the population through iterations until a termination criterion is met. By repeatedly applying the steps above, genetic algorithm explores the solution space, gradually improving the population and converging toward better solutions.[18]

It is worth noting that while genetic algorithms, like NSGA-II, can be powerful tools for finding near-optimal solutions to complex problems, they do not guarantee to find absolute best solutions in all cases because genetic algorithms work based on heuristics and probabilistic search methods. They explore the search space by iteratively evolving some candidates. The fitter individuals, *i.e.*, those with better solutions, are more likely to be selected and pass their genetic material to the next generation. In some cases, genetic algorithms may converge to an optimal or near-optimal solution, but in other cases, they may get stuck in suboptimal regions of the search space or struggle with problems that have high-dimensional or discontinuous fitness landscapes.

The effectiveness of genetic algorithms depends on several factors, including the design of the genetic operators, the fitness evaluation function, and the exploration/exploitation balance. In general, larger populations and more generations often lead to better results. However, it needs more computation power and longer computing time. Thus, to achieve a balance between computational efficiency and result accuracy, solutions provided in this study by the Pareto front, in most cases, is near-optimal, and some minor errors may exist between these solutions and the absolute optimal solution due to their heuristic nature of the algorithms.

Programming environment

The optimisation model was implemented in Pyomo which is an object-oriented open-source Python package to formulate, solve and analyse optimisation models. Pyomo modelling environment is imported to harness the Pyomo modelling capabilities which, define abstract problems, construct concrete instances, and solve specific problems using commercial and open-source solvers.[36]

Life cycle database

The study makes use of the Eco-invent database. It contains data on many sorts of processes and covers a wide range of industries and sectors. The Eco-invent database contains statistics on energy and resource consumption, air, water, and soil pollutants, and waste generated by various activities and goods.[14]

ReCiPe is utilised as a default LCA characterisation model in LCA optimisation model numerical characterisation factors embedded in ReCiPe link the input–output flows with impact categories and convert inventory to category indicators to be optimised.[15]

GUI of the toolkit

The software developed in the study provides a wide range of functionalities across four different interfaces: main window, process window, product window, and optimisation window. The toolkit's user-friendly interface, encompassing various windows and functionalities, ensures that users can seamlessly navigate through the optimisation process, modify the supply chain, customise processes and products, and ultimately make informed decisions to enhance the system's overall efficiency.

Fig. S-1 in ESI† shows the main window of the toolkit. The function bar is at the top of the interface and allows users to choose different functionalities, such as opening and saving files, changing the supply chain, and starting system optimisation. Under the function bar, users can see the structure of the supply chain.

Fig. S-2 in ESI† shows the process window. The process information box is at the top of the screen. It lets users change and customise the process. Under the information box, users can look in the table for processes that are already existing in the dataset.

Fig. S-3 in ESI† shows the product window, which can be used to configure data related to products. At the top of the window is a box for product information, which lets users change the details of the product. Also, all the product flows in the dataset are shown below. This gives users a complete picture and makes looking for and choosing a particular product flow quickly.

Fig. S-4 in ESI† shows the optimisation window, which is one of the most essential parts of the tool. Three different optimisation models exist: the weighted sum method for two-objective optimisation, the Pareto front for two-objective optimisation, and the Pareto front for three-objective optimisation. These options can be used for different optimisation, and users can choose the optimisation process based on their specific needs and goals.

Results and discussion

Case studies

The system presented in this case study is modelled using process systems engineering. Each process represents either a production process or a transmission process.

To illustrate the practical implementation of the methods, a case study focusing on electricity production in the UK is presented, considering the planning horizon of 2030. The assumption for domestic electricity consumption is based on statistical data from 2021, amounting to 109 450 GWh.[37] To align with the UK government's promise to slash emissions by 68% by the end of the decade, compared to 1990,[5] the allowable CO_2 equivalent emissions from energy supply should not exceed 65.312 million tons.[38] The consideration of the government subsidy entails the feed-in tariff scheme[39] and the price of emissions allowances at the end of 2021 [40] is used in the weighted sum method in case study (1).

Beyond greenhouse gases, ozone depletion is another major current environmental problem;[41] thus, it is also considered in the study. Three main objective patterns have been proposed. The objectives of case study (1) are to maximise profits while minimising the potential for global warming. Case study (2) adopts a similar strategy to (1), but the focus moves from translating global warming potential into economic value to identifying trade-off solutions on the Pareto front. This contrasts with the method taken in case study (1). There are two different scenarios in case study (2). In scenario (a), environmental criteria are prioritised, while profitability is more important in scenario (b). In case study (3), the potential for global warming and ozone depletion are considered simultaneously. Like case study (2), there are also two distinct scenarios.

The case study is an in-depth analysis that includes five distinct electricity generation technologies, which together form the superstructure of the entire system, visually represented in Fig. 1.

The system has diverse energy sources, each capable of producing high-voltage or low-voltage electricity. The four energy sources that produce high-voltage electricity are natural gas, heat and power co-generation, wind power, and hydroelectric power. The use of natural gas focuses on two technologies: combined cycle and conventional power plants. Furthermore, the case study includes the utilisation of heat and power co-generation, including the use of biogas and two types of natural gas plants. The study also incorporates wind power, including various turbine technologies. Three onshore turbines, each with unique power capacities, are included alongside an offshore turbine. In addition to natural gas and wind power, the case study encompasses hydroelectric power generation. Two hydroelectric technologies, pumped storage and run-of-river are included. The generated electricity needs to experience two steps of transformation, ensuring that the electricity produced by these processes meets the low-voltage requirements of households. Moreover, the case study explores an alternative avenue for electricity generation, photovoltaic technology, which directly generating low voltage electricity.

Among those energy sources considered in the case studies, natural gas prices are subject to the most significant fluctuations due to factors such as geopolitical tensions, and the uncertainty of supply and demand dynamics, which impacts planning and budgeting. To understand the sensitivity of the modelling results, we explored how the change in natural gas prices affects the selection of different energy sources for electricity generation.

Table 2 offers a complete summary of the objectives for each scenario, outlining the goals taken into consideration and the method used in each scenario.

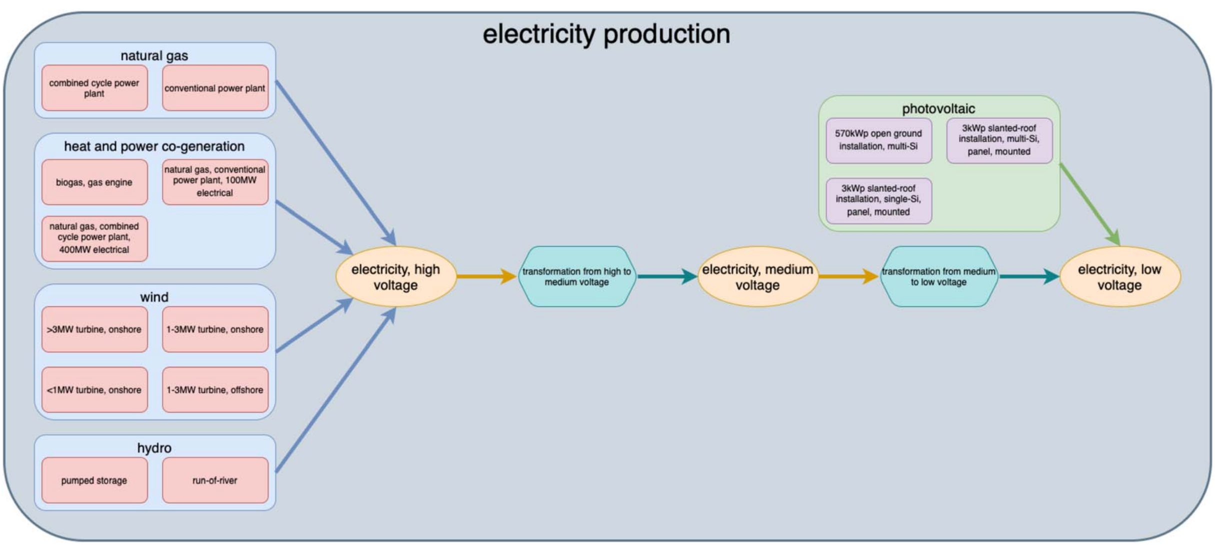

Fig. 1 Superstructure for the case study.

Table 2 Objectives of the case studies

Case study no.	Objective 1	Objective 2	Objective 3	Multi-objective optimisation method
(1)	Profit (£)	Global warming potential (GWP) (kg of CO_2 eq.)	—	Weighted sum method
(2)	Profit (£)	Global warming potential (GWP) (kg of CO_2 eq.)	—	Finding Pareto front with genetic algorithm
(3)	Profit (£)	Global warming potential (GWP) (kg of CO_2 eq.)	Ozone depletion potential (kg of CFC-11 eq.)	Finding Pareto front with genetic algorithm

Table 3 Parameters for electricity production processes

Energy source	Voltage	Revenue (£/kWh)	Feed-in tariff (£/kWh)	Profit (£/kWh)	Global warming potential (kg of CO_2 eq./kWh)	Ozone depletion potential (kg of CFC-11 eq./kWh)
Electricity production, natural gas, conventional power plant|electricity, high voltage|APOS, S	High	8.40×10^{-2}	0	8.40×10^{-2}	5.12×10^{-1}	3.59×10^{-8}
Electricity production, natural gas, combined cycle power plant|electricity, high voltage|APOS, S	High	8.40×10^{-2}	0	8.40×10^{-2}	3.50×10^{-1}	2.56×10^{-8}
Heat and power co-generation, biogas, gas engine|electricity, high voltage|APOS, S	High	8.40×10^{-2}	6.73×10^{-2}	1.51×10^{-1}	1.88×10^{-1}	1.74×10^{-8}
Heat and power co-generation, natural gas, conventional power plant, 100 MW electrical|electricity, high voltage|APOS, S	High	8.40×10^{-2}	6.73×10^{-2}	1.51×10^{-1}	4.54×10^{-1}	3.33×10^{-8}
Heat and power co-generation, natural gas, combined cycle power plant, 400 MW electrical|electricity, high voltage|APOS, S	High	8.40×10^{-2}	6.73×10^{-2}	1.51×10^{-1}	3.77×10^{-1}	2.76×10^{-8}
Electricity production, wind, >3 MW turbine, onshore|electricity, high voltage|APOS, S	High	8.40×10^{-2}	3.82×10^{-2}	1.22×10^{-1}	2.23×10^{-2}	1.81×10^{-9}
Electricity production, wind, 1–3 MW turbine, onshore|electricity, high voltage|APOS, S	High	8.40×10^{-2}	3.82×10^{-2}	1.22×10^{-1}	1.28×10^{-2}	9.12×10^{-10}
Electricity production, wind, <1 MW turbine, onshore|electricity, high voltage|APOS, S	High	8.40×10^{-2}	3.82×10^{-2}	1.22×10^{-1}	1.23×10^{-2}	6.16×10^{-10}
Electricity production, wind, 1–3 MW turbine, offshore|electricity, high voltage|APOS, S	High	8.40×10^{-2}	3.82×10^{-2}	1.22×10^{-1}	1.56×10^{-2}	8.24×10^{-10}
Electricity production, hydro, pumped storage|electricity, high voltage|APOS, S	High	8.40×10^{-2}	3.72×10^{-2}	1.21×10^{-1}	5.75×10^{-1}	6.99×10^{-8}
Electricity production, hydro, run-of-river|electricity, high voltage|APOS, S	High	8.40×10^{-2}	3.72×10^{-2}	1.21×10^{-1}	4.04×10^{-3}	2.86×10^{-10}
Electricity production, photovoltaic, 3kWp slanted-roof installation, single-Si, panel, mounted|electricity, low voltage|APOS, S	Low	9.20×10^{-2}	1.75×10^{-2}	1.09×10^{-1}	1.22×10^{-1}	1.28×10^{-8}
Electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted|electricity, low voltage|APOS, S	Low	9.20×10^{-2}	1.75×10^{-2}	1.09×10^{-1}	7.48×10^{-2}	9.01×10^{-9}
Electricity production, photovoltaic, 570kWp open ground installation, multi-Si|electricity, low voltage|APOS, S	Low	9.20×10^{-2}	1.75×10^{-2}	1.09×10^{-1}	7.65×10^{-2}	8.63×10^{-9}

Table 4 Parameters for electricity transformation processes

Transformer type	Transformation rate (%)	Profit (£/kWh)	Global warming potential (kg of CO_2 eq./kWh)	Ozone depletion potential (kg of CFC-11 eq./kWh)
Electricity voltage transformation from high to medium voltage|electricity, medium voltage|APOS, S	99.31	8.60×10^{-2}	3.70×10^{-1}	4.89×10^{-8}
Electricity voltage transformation from medium to low voltage|electricity, low voltage|APOS, S	97	9.20×10^{-2}	3.83×10^{-1}	5.53×10^{-8}

The important parameters of each technology used in the case study are outlined in Table 3. The data used to parameterise the model are derived from Eco-invent 3.7.1,[42] ReCiPe 2016 (ref. 46) and online carbon price tracker.[40]

Table 4 shows the parameters associated with the processes of voltage transformation. Eco-invent 3.7.1 (ref. 42) is used to get the information on all the processes while ReCiPe 2016 (ref. 46) is the source of the data that was utilised to calculate the environmental impacts.

Optimal solution for case study (1)

The time used for Pyomo to solve the optimisation problem is 0.02 seconds. In case study (1), where the objectives include minimising the potential for global warming and maximising profit, the optimal outcome that can be obtained is 29.11 billion pounds. This result is derived by multiplying the price of emission allowances which is 0.0746 (£/kg of CO_2 eq.), by the global warming potential to transform it into an economic value. Heat and power co-generation with biogas is used to generate all the electricity.

Optimal solutions for case study (2)

The time used to run the algorithm is 2 minutes and 54 seconds. In scenario (a), the optimal profit reaches 26.03 billion pounds, and the corresponding global warming potential is 24.62 billion kg CO_2 equivalent when the primary emphasis is placed on satisfying the demand for power consumption in household settings. In scenario (b), to follow the emission reduction goals set for 2030, the maximum profit that can be achieved through the generation of electricity increases to 44.86 billion pounds, with a global warming potential of 63.39 billion kg CO_2 equivalent. The Pareto front depicted in Fig. 2a visually represents the trade-off between the two objectives: maximising profits and minimising GHGs emissions.

The measurement for GHGs emission is the amount of CO_2 equivalent. As the amount of GHGs increase, so does the profit level. However, achieving a perfect point with low emissions and high profit is not feasible. Policymakers and business owners are tasked with selecting different points along the Pareto front based on their specific needs. In scenario (a), the points situated in the lower-left corner offer more sustainable solutions, albeit at the expense of profit. Conversely, in scenario (b), the objective is to maximise profit, the point in the top-right corner should be chosen. A compromise point is often preferred in the middle of the Pareto front to balance these conflicting objectives.

The contributions made by various energy sources are broken down in Table 5 for scenarios (a) and (b). The table provides information on the energy produced in kilowatt-hours (kWh) for different energy sources in two scenarios, (a) and (b).

In scenario (a): natural gas electricity production from a combined cycle power plant generated 5.75×10^8 kWh. Heat and power co-generation using biogas in a gas engine produced 4.22×10^8 kWh. Wind energy production from onshore wind turbines (>3 MW) produced 4.20×10^9 kWh. Wind energy production from offshore wind turbines (1–3 MW) generated 4.04×10^8 kWh. Hydro energy production from run-of-river sources generated 6.73×10^8 kWh. Photovoltaic systems with a 3kWp slanted-roof installation using single-Si panels generated 6.20×10^{10} kWh. Photovoltaic systems with a 3kWp slanted-roof installation using multi-Si panels generated 7.49×10^{10} kWh. Photovoltaic systems with a 570kWp open ground installation using multi-Si panels generated 8.39×10^{10} kWh.

In scenario (b): natural gas electricity production from a conventional power plant generated 2.30×10^6 kWh. Natural gas electricity production from a combined cycle power plant generated 3.00×10^8 kWh. Wind energy production from onshore wind turbines (>3 MW) generated 8.89×10^9 kWh. Wind energy production from onshore wind turbines (<1 MW) generated 1.02×10^{10} kWh. Wind energy production from offshore wind turbines (1–3 MW) generated 1.92×10^{10} kWh. Hydro energy production from run-of-river sources generated 1.43×10^{10} kWh. Photovoltaic systems with a 3kWp slanted-roof installation using single-Si panels generated 7.18×10^{10} kWh. Photovoltaic systems with a 3kWp slanted-roof installation using multi-Si panels generated 9.50×10^{10} kWh. Photovoltaic systems with a 570kWp open ground installation using multi-Si panels generated 9.97×10^{10} kWh. Photovoltaic systems with a 570kWp open ground installation using multi-Si panels generated 9.97×10^{10} kWh.

Fig. 3a illustrates that in scenario (a), photovoltaics was responsible for 97.33% of the total power production, whereas the other four techniques were only responsible for 2.67% of the total electricity production. In scenario (b), as shown in Fig. 3b photovoltaics contributed an overall total of 83.96% of the

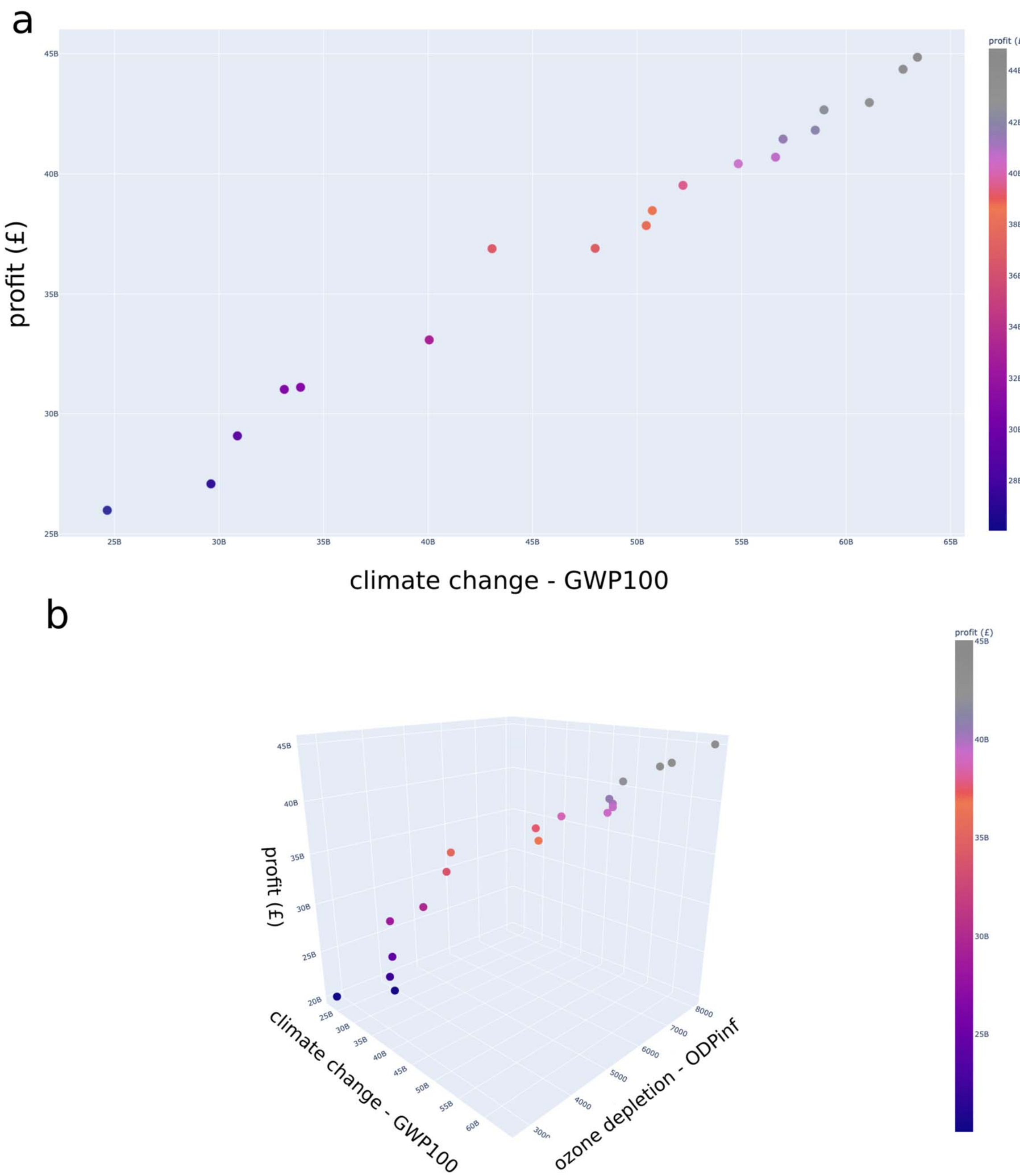

Fig. 2 Pareto front. (a) Case study 2. (b) Case study 3.

electricity, but the other four techniques only contributed 16.04% of the electricity when combined.

In scenario (a), natural gas produced 5.75×10^8 kWh (0.25%) of electricity, heat and power co-generation produced 4.22×10^8 kWh (0.17%) of electricity, wind turbines generated 4.60×10^9 kWh (1.96%) of electricity, and hydro stations produced 6.73×10^8 kWh (0.29%) of electricity. Photovoltaic produced 2.20×10^{11} kWh (97.33%) of electricity. The detailed flows are depicted in Fig. 4a.

In scenario (b), natural gas generated 3.02×10^8 kWh (0.08%) high voltage electricity, wind turbine generated 3.82×10^{10} kWh (11.62%) electricity, hydroelectric station generated 1.43×10^{10} kWh (4.34%) high voltage electricity. Solar energy produced 2.66×10^{11} kWh (83.96%) low voltage electricity. Fig. 4b depicts the flows. Fig. S-5 in ESI† depicts the impact of changing natural gas prices on energy selection. Our results suggested that in both sustainability-prioritised and profitability-prioritised scenarios, the share of natural gas sees a notable rise as the market price increases.

The findings of case study (2) demonstrate that solar power is the primary source of energy production in both (a) and (b) of the scenarios. This is mainly because photovoltaic is, in

Table 5 Contributions of different energy sources in case study (2)

Energy source	Energy produced in scenario (a) (GWh)	Energy produced in scenario (b) (GWh)
Electricity production, natural gas, conventional power plant|electricity, high voltage|APOS, S	0	2.30
Electricity production, natural gas, combined cycle power plant|electricity, high voltage|APOS, S	5.75×10^2	3.00×10^2
Heat and power co-generation, biogas, gas engine|electricity, high voltage|APOS, S	4.22×10^2	0
Heat and power co-generation, natural gas, conventional power plant, 100 MW electrical|electricity, high voltage|APOS, S	0	0
Heat and power co-generation, natural gas, combined cycle power plant, 400 MW electrical|electricity, high voltage|APOS, S	0	0
Electricity production, wind, >3 MW turbine, onshore|electricity, high voltage|APOS, S	4.20×10^3	8.89×10^3
Electricity production, wind, 1–3 MW turbine, onshore|electricity, high voltage|APOS, S	0	0
Electricity production, wind, <1 MW turbine, onshore|electricity, high voltage|APOS, S	0	1.02×10^4
Electricity production, wind, 1–3 MW turbine, offshore|electricity, high voltage|APOS, S	4.04×10^2	1.92×10^4
Electricity production, hydro, pumped storage|electricity, high voltage|APOS, S	0	0
Electricity production, hydro, run-of-river|electricity, high voltage|APOS, S	6.73×10^2	1.43×10^4
Electricity production, photovoltaic, 3kWp slanted-roof installation, single-Si, panel, mounted|electricity, low voltage|APOS, S	6.20×10^4	7.18×10^4
Electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted|electricity, low voltage|APOS, S	7.49×10^4	9.50×10^4
Electricity production, photovoltaic, 570kWp open ground installation, multi-Si|electricity, low voltage|APOS, S	8.39×10^4	9.97×10^4

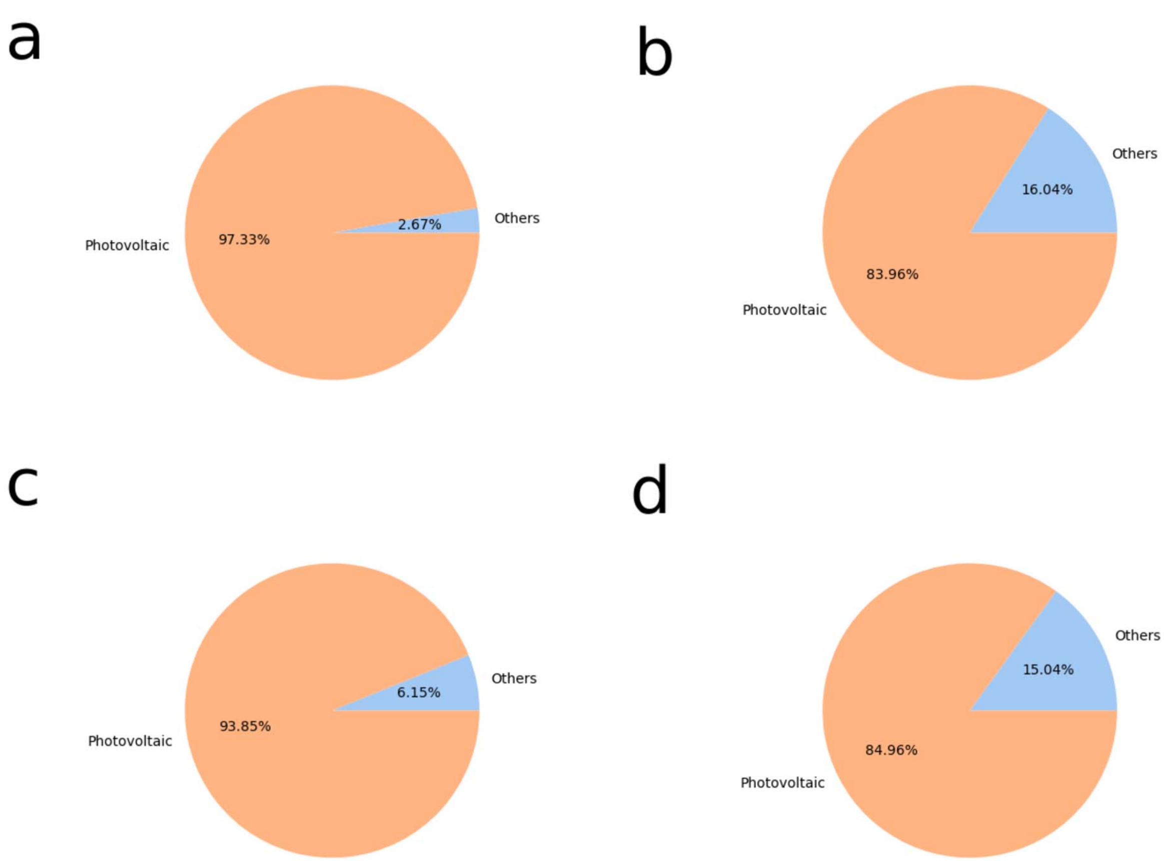

Fig. 3 Contribution of different energy sources. (a) Scenario a in case study 2. (b) Scenario b in case study 2. (c) Scenario a in case study 3. (d) Scenario b in case study 3.

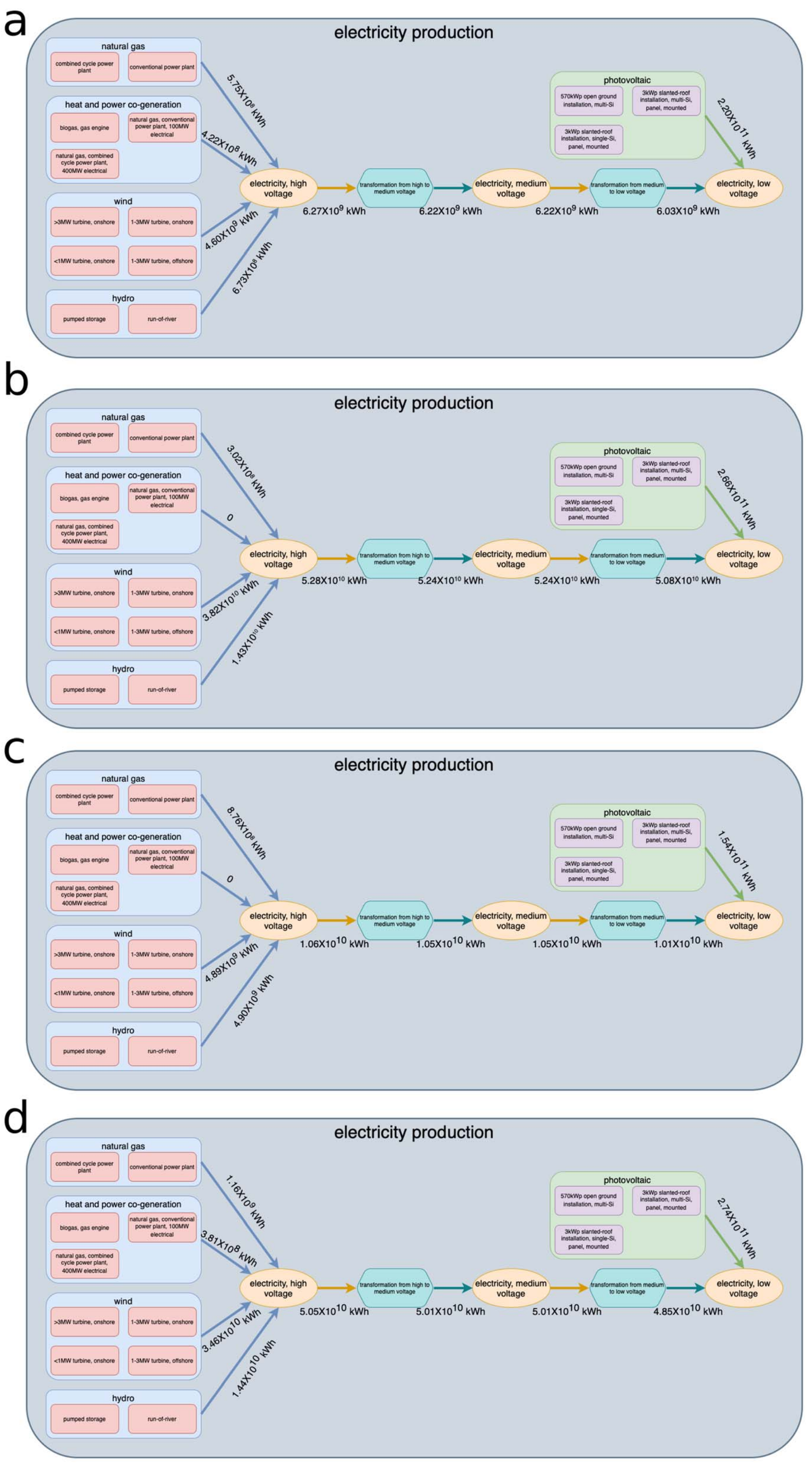

Fig. 4 Flows information. (a) Scenario a in case study 2. (b) Scenario b in case study 2. (c) Scenario a in case study 3. (d) Scenario b in case study 3.

Table 6 Contributions of different energy sources in case study (3)

Energy source	Energy produced in scenario (a) (GWh)	Energy produced in scenario (b) (GWh)
Electricity production, natural gas, conventional power plant|electricity, high voltage|APOS, S	8.76×10^2	0
Electricity production, natural gas, combined cycle power plant|electricity, high voltage|APOS, S	0	1.16×10^3
Heat and power co-generation, biogas, gas engine|electricity, high voltage|APOS, S	0	0
Heat and power co-generation, natural gas, conventional power plant, 100 MW electrical|electricity, high voltage|APOS, S	0	0
Heat and power co-generation, natural gas, combined cycle power plant, 400 MW electrical|electricity, high voltage|APOS, S	0	3.81×10^2
Electricity production, wind, >3 MW turbine, onshore|electricity, high voltage|APOS, S	0	3.33×10^4
Electricity production, wind, 1–3 MW turbine, onshore|electricity, high voltage|APOS, S	8.03×10^2	0
Electricity production, wind, <1 MW turbine, onshore|electricity, high voltage|APOS, S	5.56×10^2	0
Electricity production, wind, 1–3 MW turbine, offshore|electricity, high voltage|APOS, S	3.54×10^3	1.35×10^3
Electricity production, hydro, pumped storage|electricity, high voltage|APOS, S	2.93×10^3	6.07×10^1
Electricity production, hydro, run-of-river|electricity, high voltage|APOS, S	1.97×10^3	1.44×10^4
Electricity production, photovoltaic, 3kWp slanted-roof installation, single-Si, panel, mounted|electricity, low voltage|APOS, S	2.24×10^4	8.57×10^4
Electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted|electricity, low voltage|APOS, S	5.05×10^4	9.80×10^4
Electricity production, photovoltaic, 570kWp open ground installation, multi-Si|electricity, low voltage|APOS, S	8.13×10^4	9.06×10^4

comparison to other technologies, significantly more environmentally friendly and clean. Additionally, because it can directly create electricity at low voltage, this eliminates the need for an intermediary transformation, which reduces emissions. When profitability is prioritised, the percentage of electricity generated by photovoltaics decreases. This is because photovoltaics is not the most profitable type of electricity generation.

Optimal solutions for case study (3)

The time used to run the algorithm in case study (3) is 3 minutes 10 seconds. The optimal solutions for three-objective optimisation are presented under various assumptions. In case study (3), ozone depletion potential becomes an additional consideration. The minimal possible amount for global warming potential is 22.85 billion kg CO_2 equivalent, and for ozone depletion potential is 2778.72 kilograms of CFC-11 equivalent. At this point, the profit is 20.03 billion pounds. In scenario (b), for the UK government to meet its goals by the year 2030, the greatest profit that can be made from the generation of electricity is 45.04 billion pounds, and the potential for global warming is 63.61 billion kilograms of CO_2 equivalent and for ozone depletion is 8055.68 kilograms of CFC-11 equivalent.

In case study (3), the Pareto front is plotted in 3-D figures in Fig. 2b since there are three distinct objectives: profits, global warming potential, and ozone depletion potential. These figures illustrate that profitability increases but at the expense of higher emissions. Unlike the 2-D figure, the 3-D representation gives policymakers and business owners a broader range of choices. They can now make decisions not only based on profit and greenhouse gas emission limits but also with consideration for the second environmental category.

The contributions made by various energy sources are broken down in Table 6 for scenarios (a) and (b). The table provides data on the energy production in kilowatt-hours (kWh) for various energy sources in scenarios (a) and (b). Natural gas: in scenario (a), a natural gas conventional power plant generated 8.76×10^8 kWh, while the combined cycle power plant did not produce any energy. In scenario (b), the conventional power plant did not generate any energy, while the combined cycle power plant produced 1.16×10^9 kWh. Heat and power Co-generation: the biogas gas engine and the natural gas conventional power plant (100 MW electrical) did not produce any energy in both scenarios. The natural gas combined cycle power plant (400 MW electrical) generated 3.81×10^8 kWh in scenario (b) but no energy in scenario (a). Wind: wind energy production from onshore turbines (>3 MW) did not generate any energy in scenario (a) but produced 3.33×10^{10} kWh in scenario (b). Onshore turbines with capacities of 1–3 MW and <1 MW generated 8.03×10^8 kWh and 5.56×10^8 kWh, respectively, in scenario (a) but no energy in scenario (b). Offshore wind turbines (1–3 MW) produced 3.54×10^9 kWh in scenario (a) and 1.35×10^9 kWh in scenario (b). Hydro: the pumped storage hydro system generated 2.93×10^9 kWh in scenario (a) and 6.07×10^7 kWh in scenario (b). The run-of-river hydro system produced 1.97×10^9 kWh in scenario (a) and 1.44×10^{10} kWh in scenario (b). Photovoltaic: slanted-roof installations with single-Si panels generated 2.24×10^{10} kWh in scenario (a) and 8.57×10^{10} kWh in scenario (b). Slanted-roof installations with multi-Si panels produced 5.05×10^{10} kWh in scenario (a) and 9.80×10^{10} kWh in scenario (b). Open ground installations with multi-Si panels generated 8.13×10^{10} kWh in scenario (a) and 9.06×10^{10} kWh in scenario (b).

In scenario (a), natural gas, wind power, and hydropower produced 8.76×108 kWh (0.48%), 4.89×10^9 kWh (2.83%), 4.90×10^9 kWh (2.83%) high voltage electricity, respectively. Solar panels generated 1.54×10^{11} kWh (93.85%) of electricity. The detailed flows are shown in Fig. 4c. The overall contribution of photovoltaics to the generation of electricity is shown to be 93.85% in Fig. 3c, whereas the combined contribution of the other four technologies to the generation of energy is only 6.15%. In scenario (b), natural gas generated 1.16×10^9 kWh (0.33%), heat and power co-generation produced 3.81×10^8 kWh (0.10%), wind produced 3.46×10^{10} kWh (10.33%), and hydro generated 1.44×10^{10} kWh (4.28%) high voltage electricity. Photovoltaic produced 2.74×10^{11} kWh (84.96%) low voltage electricity. The detailed flows are displayed in Fig. 4d. As seen in Fig. 3d, photovoltaics generated 84.96% of the total electricity, while the other four technologies combined only produced 15.04%. Fig. S-6 in ESI† shows the effects of rising natural gas price on energy choice. In both scenario (a) and scenario (b), the contribution of natural gas experiences a significant increase as its prices go up.

The findings of case study (3) indicate that solar energy is the primary source utilised in both (a) and (b) of the possible scenarios. This is mainly because photovoltaic is a comparatively more environmentally friendly and clean approach than others. Additionally, it can immediately generate low voltage power, avoiding the emission caused by the intermediary transformation process. Because photovoltaic is not the most profitable power generation, this method's electricity generation percentage drops slightly when profitability is a higher priority.

Conclusions

This study integrates LCA and optimisation, and presents a LCA optimisation toolkit, enabling solutions to account for environmental and economic objectives simultaneously. Implementing multi-objective optimisation in this setting facilitates the discovery of multiple Pareto-optimal alternatives that can improve the design and operation.

The effectiveness of the suggested approach and accompanying tools are tested *via* a case analysis concentrating on electricity generation within the UK. In the first case study, the environmental and economic objectives are combined into a single goal using weighted sum methods, with emission allowances' price as the weight. This approach yields an optimal solution that maximises profit. In the remaining two case studies, genetic algorithms are employed to obtain the Pareto front, enabling the identification of multiple compromise solutions. These solutions include achieving the minimum emissions necessary to meet domestic electricity consumption demand and maximising profit in the years 2030 while complying with the net zero targets of the UK government.

As a result, decision-makers and other stakeholders can gain vital insights into the possible outcomes that can be achieved by pursuing a variety of tactics. Developing a sustainable and economically viable energy landscape in the UK is possible by taking a comprehensive and informed approach to planning and optimising electricity generation. This approach should take into consideration a variety of aspects, including profit, reductions in emissions, and the effects on the environment. The case study exemplifies the practical application of the suggested methodology, thus emphasising its efficacy in addressing practical issues related to electricity generation and mitigation of emissions.

Striking the right balance between environmental responsibility and profitability is a complex and multifaceted challenge that businesses must confront in pursuing sustainable success. This analysis helps identify the optimal solutions that align with the goals and priorities of stakeholders involved in the electricity production system.

The results demonstrate the importance of considering various assumptions and their impact on outcomes. For businesses with a solid commitment to minimising their environmental impact, once they have met the household electricity consumption requirements, it becomes imperative for them to curtail their production to the absolute minimum, which is crucial because an increase in production directly translates to higher emissions, which is in direct contradiction to their sustainability goals. On the other hand, businesses that prioritise profitability face a different set of considerations. Maximising electricity production is advisable for them as it directly correlates with increased profits. By ramping up production levels, they can become more profitable. However, there is also a limit to how much they can produce because they must balance maximising profitability and adhering to the government's greenhouse gas emissions regulations.

The results illustrate that solar power offer a sustainable solution as predominant energy source. This preference arises primarily from the notably superior environmental performances of photovoltaic technology compared to other alternatives. Furthermore, its capacity to generate electricity at low voltage decentralised energy systems directly eliminates the necessity for an intermediary transformation, thereby mitigating emissions. This finding aligns with other previous research findings published on energy systems. Developing solar module production has been proved to result in 6.7% in emission reductions in Colombia,[47] while the deployment of distributed photovoltaics in countries like Bangladesh, which are endowed with rich solar resources, can be conducive to both economic and environmental aspects.[48] Other studies on global south energy systems also highlighted that implementing solar water heating (SWH) systems in Ghanaian hotels using the country's solar potential could lead to substantial financial savings, reduced reliance on fossil fuels, and lower carbon emissions, making it an attractive and viable investment for hotel owners.[49] Another study illustrates that a novel air conditioning system powered by solar energy can enhance vehicle fuel efficiency, demonstrating a 25% reduction in fuel consumption compared to conventional systems, along with improved cooling and heating capabilities; additionally, the solar-powered system leads to decreased harmful engine emissions.[50]

Several research areas have emerged from current study which are worth further exploration in future work. Firstly, our life cycle optimisation model can be further configured to consider open-loop or closed-loop waste (in liquid, gas, solid phases) recovery to inform circular-economy decisions. Secondly, in a centralised supply chain, key decision-making regarding procurement, production, and distribution are made at a central location or by a central authority within the organization. By contrast, in supply chains characterized by decentralised decision-making, each participant possesses the autonomy to make its own choices. Consequently, this introduces a multi-player dimension to the design of the supply chain, presenting research challenges in both modelling and computational aspects. Decentralised supply chain optimisation problems can be addressed by various approaches *e.g.*, game theory, agent-based simulation. In our previous research, we have explored both approaches.[51–53] We have developed a mixed integer programming optimisation model and implemented Nash equilibrium to explore the solutions at decentralised multi-echelon supply chain levels where multiple nodes across supply chains have been considered *e.g.*, resource suppliers, manufacturers, distributors, governments, and finance sectors.[51] We have also developed an approach to couple agent-based simulation and mathematical optimisation to simulate the behaviours of each node and optimise the individual solutions across biofuel supply chains in global South.[52,53] In our future research, we will build upon the currently developed life cycle optimisation tool to explore further centralised *vs.* decentralised supply chain optimisation problems.

In addition, the life cycle optimisation presented in this study holds significant potential for global decision-making on net-zero path. One of the key challenges on the path to net zero is to take accountability for both direct and indirect GHG emissions. This challenge arises from the imbalance between developed nations and developing nations based on their historic greenhouse emissions and the lack of consideration of this fact in global policy making. It is important to transition towards fairer product-based emissions accounting where emissions and accountability are assigned over the entire value-chain across countries globally. A life cycle optimisation approach can help to form digital carbon passports and systems underpinned by data-rich networks and offer solutions to currently fragmented carbon market globally. In addition, current LCA and carbon reporting, which are cost-intensive and constrained by delayed inventory reporting and data gaps, only allows for retrospective carbon counting and data analyses. This calls for virtual value chains underpinned by digital twins to represent the physical systems and enable real-time data update and harness computational power. Thus, emerging research direction is to develop collaborative system-wide LCA optimisation platform to incorporate real-time data collection/analyse and digital-twin powered value chains and allow responsive optimisation. Such future research would enhance accountability and traceability of carbon and environmental profiles and support real-time decision-making based on prospective virtual representations.

Conflicts of interest

There are no conflicts to declare.

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