

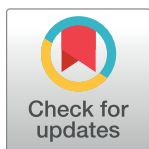
REVIEW

Optimization and decision support models for deploying negative emissions technologies

Maria Victoria Migo-Sumagang^{1,2}, Kathleen B. Aviso¹, Dominic C. Y. Foo³, Michael Short⁴, Purusothmn Nair S. Bhasker Nair³, Raymond R. Tan^{1*}

1 Department of Chemical Engineering, De La Salle University, Manila, Philippines, **2** Department of Chemical Engineering, University of the Philippines Los Baños, Laguna, Philippines, **3** Department of Chemical and Environmental Engineering/Centre of Excellence for Green Technologies, University of Nottingham Malaysia, Selangor, Malaysia, **4** Department of Chemical and Process Engineering, University of Surrey, Surrey, United Kingdom

* raymond.tan@dlsu.edu.ph



Abstract

Negative emissions technologies (NETs) will be needed to reach net-zero emissions by mid-century. However, NETs can have wide-ranging effects on land and water availability, food production, and biodiversity. The deployment of NETs will also depend on regional and national circumstances, technology availability, and decarbonization strategies. Process integration (PI) can be the basis for decision support models for the selection, planning, and optimization of the large-scale implementation of NETs. This paper reviews the literature and maps the role of PI in NETs deployment. Techniques such as mathematical programming, pinch analysis (PA), process graphs (P-graphs), are powerful methods for planning NET systems under resource or footprint constraints. Other methods such as multi-criteria decision analysis (MCDA), marginal abatement cost curves, causality maps, and machine learning (ML) are also discussed. Current literature focuses mainly on bioenergy with carbon capture and storage (BECCS) and afforestation/reforestation (AR), but other NETs need to be integrated into future models for large-scale decarbonization.

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Author summary

Radical approaches will be needed to deal with the ongoing climate crisis. In addition to the reduction of greenhouse gas emissions through strategies such as energy conservation or decarbonization of electricity, negative emissions technologies (NETs) that remove carbon dioxide from the atmosphere will also have to be commercialized. These technologies can offset both historical greenhouse gas emissions as well as residual emissions from sectors that are inherently hard to decarbonize. However, the rapid scale-up of NETs poses the risk of unintended consequences due to their need for energy, land, water, nutrients, and other resources. These requirements also translate to incremental cost and social acceptability aspects of carbon drawdown options. The evaluation of many alternatives is also problematic due to the uncertainties inherent in new technologies. This paper surveys the emerging literature on decision support models that have been developed to deal with these issues and facilitate the large-scale deployment of NETs.

Introduction

Negative emissions technologies (NETs) will be needed to achieve the global net-zero emission target by mid-century [1]. NETs remove CO₂ from the atmosphere and transfer it to other physical or biological compartments [2]. The drawback of NETs is the potential effects on biogeochemical cycles that lead to adverse environmental impacts [3]. The scale and timing of NETs deployment will depend on the regional and national circumstances, technology availability, and level of decarbonization of different sectors [1]. Hence, computer-aided decision support for NETs deployment is an important research area. Process integration (PI), a branch of process systems engineering (PSE), offers various methods for such applications.

PI is defined as “a holistic approach to design and operation that emphasizes the unity of the process” [4] and focuses on the efficient use of resources and the reduction of pollution [5]. Two groups of techniques developed in PI are pinch analysis (PA) and mathematical programming (MP) [5]. PI techniques were first used for heat recovery system design in process plants [6]. Mass integration was later developed by capitalizing on the structural similarity of heat and mass transfer [7]; PI principles were extended to CO₂ emissions reduction through carbon-constrained energy planning with tools such as carbon emissions pinch analysis (CEPA) [8]. Combining PI with artificial intelligence (AI) is also a promising area [9].

PI models can play an important role in high-level policy decision analysis to fight climate change [10]. Integrated assessment models (IAMs) remain critical in emissions reduction analysis, but they should be supplemented with other modeling approaches [11]. In particular, there is a need for optimization models to prescribe normative courses of action rather than merely describing the results of predefined scenarios [12]. PI models can therefore supplement IAMs in planning the large-scale implementation of NETs.

A keyword map based on a Scopus database search (using the search terms “negative emissions” or “carbon dioxide removal” and the techniques, “optimization,” “mathematical programming,” “linear programming,” “pinch analysis,” “marginal abatement cost,” “p-graph,” “multi-criteria decision analysis,” and “machine learning” until the year 2022 is shown in Fig 1. The sizes of the nodes indicate the frequency of occurrence. Five thematic clusters of topics based on content [13] can be seen in different colors, namely, carbon dioxide removal and optimization (blue), climate change and GHG (red), carbon capture and biomass bioenergy (green), negative emissions (yellow), and life cycle assessment (LCA) (violet). The keyword “process integration” is found under the red cluster but is linked with all the other thematic clusters, indicating that PI is an emerging topic that warrants attention.

Early literature reviews on NETs assess their technological readiness, costs, and carbon dioxide removal (CDR) potentials [14]. The biophysical limits of NETs were also evaluated based on multiple footprints [15]. A comprehensive report evaluated NETs based on costs and potentials as well as co-benefits, social acceptance, implementation barriers, and readiness [2]. A three-part review series that emphasized the importance of NET portfolios assessed the research landscape [16], costs and side impacts [17], and commercialization prospects [18]. NETs have been evaluated using the United Nations Sustainable Development Goals (UN SDGs) [19] and LCA [20]. Despite the extensive literature on NETs, no reviews have been found on the optimization and decision support models for their deployment.

This paper addresses this gap in the literature by giving a state-of-the-art survey of the optimization and decision support models for NETs, with an emphasis on PI-based techniques. The rest of the paper is organized as follows. The next section gives an overview of NETs. Subsequent sections discuss the different modeling approaches and applications in NETs depending on the task. The final section gives the conclusions and future research outlook.

Table 1. Overview of NETs.

Capture method	NET	Description	Co-benefits	Limitations	Risks
Biological	AR	Increasing the forest area to enhance the carbon sink [33]	Food, fuel, and fiber production, air quality and water regulation, recreation, and biodiversity improvement [34]	Land and water availability, permanence, and sink saturation [35]	Albedo effect, biodiversity and food security [35]
	WR	Restoration of wetlands to enhance the anaerobic storage of dead organic matter [36]	Prevent floods, filter pollutants from air and water, improve biodiversity, and provide recreation, fish, and shrimp [36]	Difficulties in restoring, permanence, and sink saturation [36]	CH ₄ emissions, albedo effect [36]
	SCS	Applying land management practices that increase the carbon content of the soil [37]	Soil enhancement and improvement of soil biodiversity [38]	Fertilizer supply, permanence, and sink saturation [37]	N and P utilization, increase in N ₂ O emissions [37]
	BC	Thermochemical conversion of organic matter under low or zero oxygen conditions to produce char, then storing it in soil or away from the atmosphere [39]	Agricultural waste management, energy source, N ₂ O and CH ₄ emissions reduction, soil enhancement, pollution adsorption, and soil biodiversity improvement [39]	Sustainable biomass supply, suitable soils for storage, sink saturation [39]	Land-use change, albedo effect, competition for biomass [39]
	BECCS	Bioenergy production from the combustion of renewable biomass, then the CCS of the exhaust CO ₂ from the combustion process [40]	Bioenergy production [40]	CO ₂ storage, sustainable biomass supply, land and water availability, suitable facilities [41]	Land-use change, food security and biodiversity, competition for biomass, albedo effect, CO ₂ leakage [40]
	OF	Application of nutrients (phosphates, nitrates, and iron) to the ocean surface to enhance the photosynthesis by phytoplankton and using the ocean's "biological pump" to move the biomass deep in the ocean [42]	No known co-benefits aside from carbon sequestration	Fertilizer supply [42]	Unknown impacts on marine biodiversity, toxic algal blooms [42]
Geochemical/chemical	EW	Enhancing the natural weathering of rocks by crushing, grinding, and spreading alkaline materials that use CO ₂ and release metal, carbonate, and bicarbonate ions [43]	Increased nutrient availability, higher quality soils, reduced erosion rates, reversal of soil and ocean acidification, strengthens crops' resistance to pests [44]	Finite solubility of silicic acid, availability of suitable land, energy supply [43]	Ultrafine particles may cause pulmonary diseases, mining impacts [45]
	OA	The addition of calcium hydroxide or calcium oxide to ocean surface waters accelerates the uptake of CO ₂ from the atmosphere [46]	Reversal of ocean acidification [46]	Lime supply, energy supply [46]	Uncertain impacts on marine biodiversity [47], mining impacts [46]
	DACCS	Capturing low concentration CO ₂ from the atmosphere using supported amines in solid form, wet scrubbing systems based on calcium or sodium cycling technology, or other technologies, then storing the captured CO ₂ in geological reservoirs, minerals, or low carbon concrete [48]	No known co-benefits aside from carbon sequestration	CO ₂ storage, energy supply [48]	High CO ₂ penalty if fossil fuels are used, high capital costs [41]

AR, afforestation/reforestation

BC, biochar

BECCS, bioenergy with carbon capture and storage

CCS, carbon capture and storage

DACCS, direct air carbon capture and storage

EW, enhanced weathering

NET, negative emissions technology

OA, ocean alkalization

OF, ocean fertilization

SCS, soil carbon sequestration

WR, wetland restoration.

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As with any large-scale technology, NETs are not without risks. They have biogeochemical and technological limits and may cause unintended side effects [24]. The possible negative consequences of BECCS and AR were reiterated in AR6, as the maladaptation of BECCS and AR may result in risks such as damage to biodiversity, water and food security, and livelihoods [28]. NETs also have uncertain performance and costs due to immaturity [29]. NETs strategies should be tailored to fit national or regional targets and conditions [1]. Aside from resource constraints, NETs are also bound to temporal constraints such as technological readiness and time-varying peak CDR potentials [17,30]. Inherent uncertainties in the scale and permanence of CDR should also be considered [31]. These aspects call for careful planning of NETs deployment [32]. NETs portfolios optimized for local conditions can be more sustainable [17]. Fig 2 illustrates the range of available NETs and the resources potentially needed to achieve CO₂ sequestration. Portfolio optimization models can be used to prescribe the mix of NETs to maximize CDR given economic and environmental constraints [12].

Optimization of NETs deployment

Mathematical programming models

MP models consist of an objective function subject to constraints in the form of equations, inequalities, and variable specifications [49]. They can handle complex, large-scale problems when properly formulated and structured. IAMs, which are based on the MP framework, optimize or simulate the global energy and other GHG-emitting systems [11]. Most IAM studies focus on BECCS due to its flexibility in transitioning energy systems to net-zero emissions [25]. It is also common to run IAMs as standalone energy systems to determine the optimum energy mix [11]. For example, a study investigated the impact of BECCS on the global energy mix using a linear programming (LP) optimization model [50]. Similar studies have been done for specific countries such as Japan [51] and the Netherlands [52]. Another study used an energy systems model to minimize the overall system cost while modeling complex carbon flows with fossil energy and biomass-based CCS/CCUS [53].

Most IAMs only focus on BECCS and AR applied individually [54]. Only 1 study to date simulated a NETs portfolio composed of BECCS, DACCS, AR, and EW, and concluded that a balanced portfolio is best from a regional perspective [55]. A review paper argues that IAMs should be supplemented by other models and analytical approaches to consider social and technical perspectives as well as local energy system conditions [11].

In PSE literature, models and algorithms are developed to find the optimum system configuration [56]. For instance, value chain optimization that considers the energy, water, food, and carbon nexus has been reported in NETs literature. Multiple conflicting objectives occur in such models, necessitating analysis of the Pareto front [57]. An example of a multi-objective NETs value chain optimization MP is the Modeling and Optimization of NET (MONET) [58]. The framework was applied to BECCS to generate the optimal supply chain by minimizing land and water use and maximizing CDR and electricity generation [58]. The framework was also demonstrated in a global BECCS network [59] and for national scenarios in the United Kingdom [60] and Qatar [61]. Another approach is life cycle optimization, which combines life cycle impact analysis and MP. This approach was demonstrated for the multi-objective optimization of a BECCS supply chain [62].

PI models are also used in optimizing the supply chains of NETs other than BECCS. In contrast with IAMs, these models are prescriptive rather than descriptive. The first paper on the optimal planning of negative emissions BC networks used a mixed-integer linear programming (MILP) model to maximize CDR by matching sources and sinks [63]. A subsequent study extended this model by adding an economic objective function and by considering the

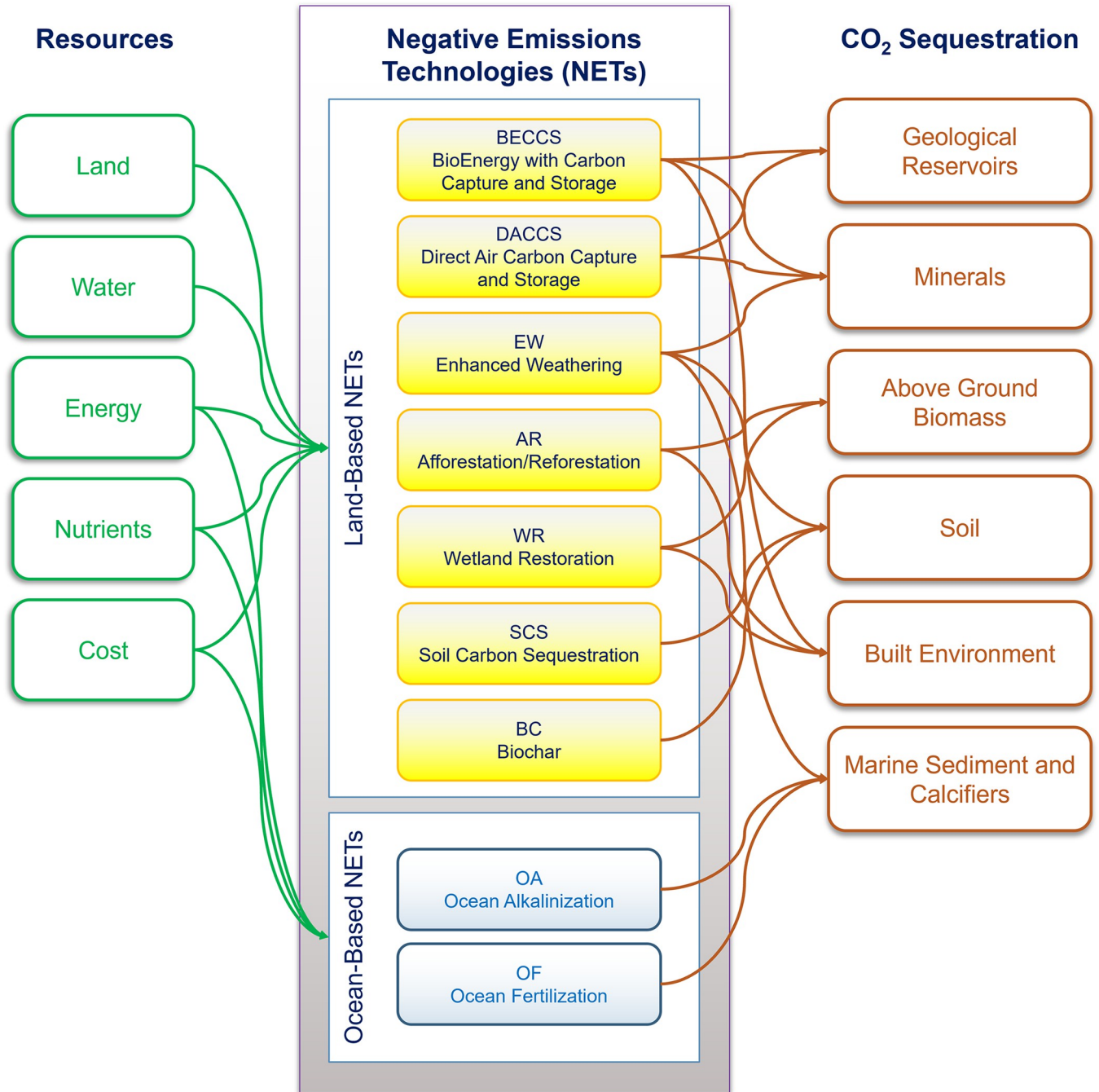


Fig 2. Superstructure for the optimization of NET portfolios. Alternative NETs rely on different physical, chemical, or biological mechanisms to sequester carbon. Each option will incur a characteristic cost and environmental footprint profile per unit of negative emissions. Portfolio optimization models can be used to prescribe the mix of NETs to maximize negative emissions given the economic and environmental constraints. NET, negative emissions technology.

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quality of the receiving soils as a sink [64]. BC systems were further explored by generating near-optimal solutions using integer cuts [65] since these solutions may exhibit desirable properties not reflected in MPs [66]. A hybrid renewable energy system with BC production was optimized in another bi-objective model that maximizes both cost and CDR [67]. The BC network was further improved by considering higher resolution constraints (CDR, and land,

water, and nutrient footprints), costs, and transport network topology [68]. MP models have also been applied to EW networks. An LP model for maximizing EW CDR by matching rock-crushing plants with rock application sites under temporal constraints was developed [69]. Models have also been proposed for the optimal design of EW networks using alkaline industrial waste in Taiwan [70] and mainland China [71].

MPs have also been proposed for integrating NETs into existing systems. For example, indirect biomass co-firing was modeled in existing coal-fired power plants wherein BC is co-produced and applied to the soil for negative emissions [72]. Another study included negative emissions BC production in optimizing combined heat and power systems with renewable (biomass and solar) energy sources [73]. A study optimized networks of ethanol biorefineries and CCS plants in the United States for total cost using integer programming [74]. Polygeneration systems, which deliver combined cooling, heating, and power, can be integrated with a negative emissions desalination process based on OA [75] while considering hourly variations in product demand and electricity price [76].

There are few PI models in the literature that consider NET portfolios. An MP model integrated BC and EW in the same system and capitalized on the synergistic relationship between the 2 NETs [77]. Another LP model optimized a NETs portfolio with AR, SCS, BECCS, BC, EW, and DACCS by evaluating the environmental footprints of each technology [78]. This approach gives the optimum NETs mix by minimizing the total cost using the Planetary Boundaries as constraints [79]. Accounting for nutrient flows in biological NETs is also critical since phosphorous is a non-renewable resource; also excess fertilizer use causes eutrophication, while excess nitrogen generates nitrous oxide (N_2O), a potent GHG [79]. The study was extended to an MILP model by considering the synergistic resource interactions between NETs [80].

MP is used in energy system models and value chain optimization commonly involving BECCS and is utilized in PI models involving BECCS, BC, EW, and rarely OA. The models usually consider cost, energy, carbon, land, and water footprints but rarely nutrient footprints. Multi-footprint models are also rare. Since NETs are commonly modeled individually, there have been few attempts to evaluate their synergistic or antagonistic interactions. Although MP is useful for detailed modeling, they have the drawback of poor interactivity when used for decision support. In the next section, alternative interactive methods will be discussed.

Graphical and algebraic pinch analysis extensions

In MP models, the optimization procedure is inherently detached from the thought processes of the decision-maker [81]. In contrast, interactive methods provide critical insights and visualization that are important in the first steps of decision analysis [82]. For example, CEPA has been extended to the planning of CCS systems [83] and more recently to NETs deployment planning (see Fig 3A; [84]). Derivative graphical [84,85] and algebraic techniques [86] have been proposed for the optimum deployment of NETs. A CEPA study of the UK's decarbonization concluded that net-zero emissions can be achieved with BECCS [87]. CEPA has also been applied for planning individual NETs such as BC [88] and EW networks [89]. Graphical PA techniques can also be replaced with mathematically equivalent algebraic procedures for easier implementation using spreadsheets [56].

Another graphical technique, known as the marginal abatement cost (MAC) curve, was originally developed in the 1980s [90]. MAC curves were popularized by McKinsey & Company to identify global cost-effective GHG emissions reduction solutions [91]. Model-based MAC curves that run alongside IAMs have also been used in NETs analysis; MAC curves for reforestation and avoided deforestation were generated using economic models [92]. Another

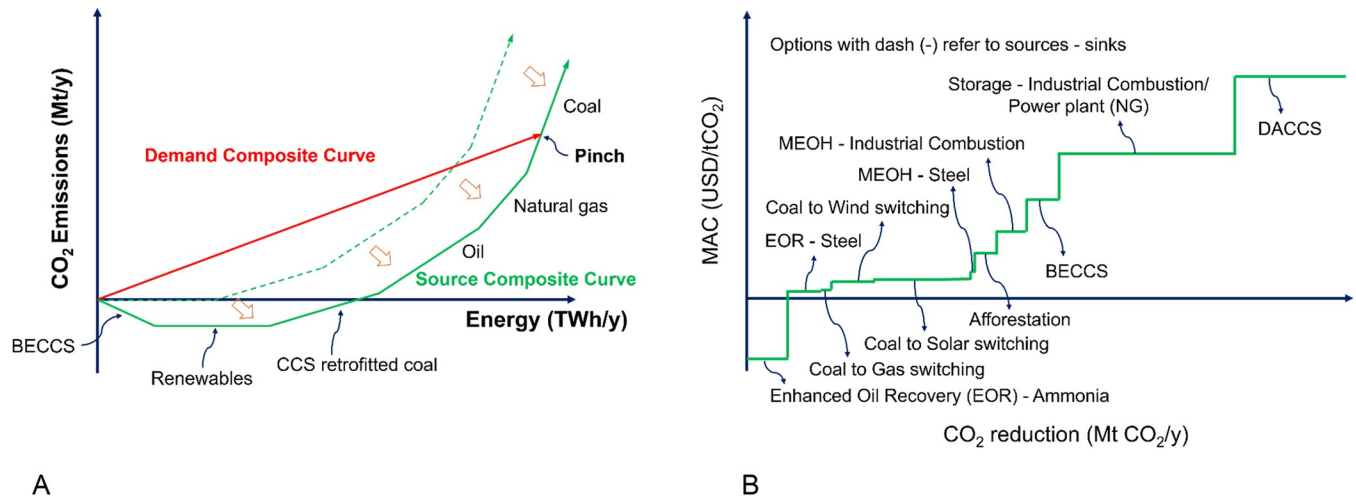


Fig 3. Graphical approaches in the optimization and prioritization of NETs deployment. (A) CEPA adapted from [84] and (B) extended MAC curve adapted from [95]. CEPA, carbon emissions pinch analysis; MAC, marginal abatement cost; NET, negative emissions technology.

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study examined the effect of BECCS on the overall system cost and MACs using energy and economic system models [93]. MAC curves were used with an energy model to select cost-efficient emissions reduction measures including biomass co-firing and CCS in Indonesia [94]. Expert-based MACs have been supplemented with algebraic targeting methods and other improvements. A minimum MAC approach, which is a hybrid graphical and algebraic targeting technique, was developed and has been illustrated in decarbonization planning as shown in Fig 3B [95].

The graphical approaches have focused on optimizing cost, energy, and carbon footprints. Demonstrating these tools on other footprints such as land, water, and nutrients can provide key insights on NETs deployment, but this remains as a research gap in the literature. Both MP and graphical approaches are powerful tools for NETs decision support. The next section discusses multi-criteria decision analysis (MCDA) techniques for ranking NETs.

Multi-criteria decision analysis techniques

In addition to quantifiable techno-economic criteria, it is also important to consider other intangible aspects of NETs, such as social acceptance, feasibility, secondary impacts, and co-benefits [96]. MCDA techniques are useful tools for the selection and prioritization of NETs considering these indicators. A study combined 2 popular MCDA methods, the analytic hierarchy process (AHP) [97] and the technique for order preference by similarity to ideal solution (TOPSIS) [98] to rank NETs based on technical readiness, potential capacity, cost, and energy requirement [99]. Another study used MCDA to evaluate various NETs based on feasibility, effectiveness, and side impacts [30]. A neutrosophic data envelopment analysis (NDEA) model was developed to rank NETs based on environmental footprints, costs, and the albedo effect [100]. A graphical decision-making tool based on a “2 × 2” framework to assess the regional value of NETs was proposed [101]. This approach maps options using “zero-carbon availability” and “benefit-cost” as the horizontal and vertical axes [101].

MCDA techniques provide decision support for ranking NETs based on hard and soft criteria. Miscellaneous decision support tools for NETs deployment will also be discussed in the next section.

Miscellaneous techniques

Machine learning (ML), which is a subset of AI, can handle tasks such as prediction, forecasting, or classification. ML techniques, which include random forests, support vector machines, and artificial neural networks, have been recently applied in NETs. Random forests were used to predict the yields of BC from slow pyrolysis, and then, the results were further subjected to LCA and economic analysis [102]. The same ML approach was used to predict the product yields and characteristics using hydrothermal treatment of different biomass feedstocks coupled with CCS [103]. A decision framework was developed to evaluate the economic feasibility of BECCS through a combination of ML, LCA, and economic analysis and was demonstrated in a regional case study [104].

Rule-based ML approaches have also been used for the classification of geological CO₂ storage sites for BECCS or DACCS. These techniques that generate if-then rules have the advantage of inherent interpretability [105]. A study developed a rough set-based ML technique [106] to predict reliable CO₂ storage sites. The rule-based classifier was trained on a dataset of CO₂ storage sites with known geological attributes [107]. A rule-based hyperbox classifier trained using an MILP model has also been developed to identify secure CO₂ storage sites [105].

The process graph (P-graph) framework was originally developed to solve process network synthesis (PNS) problems [108] and is now used to solve a range of analogous problems [109]. It has the advantage of being able to exhaustively generate optimal and near-optimal solutions, which is important in decision-making since the optimal solutions are sometimes impractical and less robust than the suboptimal solutions [66]. P-graph models have been proposed for planning NETs systems based on BC application [110] and OA [111]. An inductive MCDA technique based on P-graph has been proposed to rank NETs [112]. The approach is similar to ML in that it relies on learning from examples. Implementation of NETs considering government–industry interactions was modeled as a Stackelberg game and solved with P-graph [113]. P-graph was also used to generate causality maps to show complex influences between NETs barriers and enablers [114].

The various modeling approaches involving NETs presented in this work and the techniques matched with the tasks are summarized in Table 2. Note each has its own applicability, strengths, and limitations.

Table 2. NETs modeling techniques and the tasks involved.

	Simulation	Optimization	Selection	Prioritization	Classification	Examples
MP	✓	✓	✓	✓	✓	[60–67,69–80,82]
PA	✓	✓	✓	✓		[85–91]
MAC curves		✓	✓	✓		[94–97]
MCDA			✓	✓		[32,101]
ML	✓				✓	[105–108,110]
P-graph	✓	✓	✓	✓		[114–118]

MAC, marginal abatement cost
 MCDA, multi-criteria decision analysis
 ML, machine learning
 MP, mathematical programming
 PA, pinch analysis
 P-graph, process graph.

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Uncertainty analysis

Epistemic uncertainties due to a lack of knowledge of the system are common in emerging technologies like NETs [9]. Examples of epistemic uncertainties in NETs planning include uncertainties in performance and cost [17,29], resource constraints [115], permanence [16,116], and social acceptability [2,117]. Stochastic uncertainties, which arise from the randomness of the system, are also present in NET planning in the form of variations in the parameters [117]. Fuzzy, stochastic, and robust programming techniques can be used to deal with these uncertainties [118].

Fuzzy decision-making seeks the “confluence” of the fuzzy goals with the fuzzy constraints in a given problem [119]. Fuzzy MP can address epistemic uncertainties of model parameters [120] and perform non-compensatory, multi-objective optimization [77]. It has been widely applied in sustainable energy technologies [121]. Fuzzy optimization has been demonstrated on NETs such as BC from biomass co-firing [72], EW networks [70], integrated EW and BC networks [77], and multi-footprint optimization of NET portfolios [80].

Post-optimization sensitivity analysis can also be done to evaluate the parametric uncertainties in NETs. For example, this approach was applied to negative emission desalination by varying the price of treated brine [76] and to BC by varying CDR targets [68]. Optimized NETs portfolios were also subjected to sensitivity analysis by evaluating the parametric uncertainties in the resource constraints [78]. Monte Carlo simulation has been used for the analysis of suboptimal solutions generated using integer cuts [66] or P-graph [109]. This two-step approach has also been reported in the literature to identify robust emissions reduction strategies [29] and robust CCS networks [122].

Conclusions and future research outlook

Planning for NETs deployment will play a significant role in achieving global climate goals [12]. Although the climate change mitigation benefits of NETs deployment are global, the costs, risks, and environmental impacts (or co-benefits) may be geographically localized. Various modeling approaches have been surveyed in this work. Ubiquitous IAM models need to be supplemented with other computing tools capable of prescribing optimal decisions [11]. PI techniques can bridge this gap by reducing resource consumption, carbon footprint, and waste [4] in the implementation of NETs. The following specific research gaps and opportunities are identified:

- Whereas IAMs have focused on BECCS and AR [54], there is a research gap in models involving other NETs. PI techniques can supplement IAMs by modeling other NETs such as BC, EW, and OA. PI tools can also be applied to carbon management networks and industrial processes involving NETs.
- There are very few studies on NETs portfolios on smaller scales, even if their sustainability benefits are clear [16]. PI tools can support the optimization of NETs portfolios on regional scales to ease the impact of individual technologies and hedge risks of underdevelopment of individual technologies.
- Multi-objective studies should consider cost, CDR, and environmental footprints [57]. Nutrients (nitrogen and phosphorous) footprints of biomass-based NETs need to be examined more closely relative to the Planetary Boundaries [79].
- Graphical approaches like PA and MAC have been extended to NETs considering cost and CDR. These tools need to be improved to be able to handle other aspects of NETs deployment.

- Multi-period models are available in the PI NETs literature, but they only consider short timeframes [76]. Future NETs planning models need to account for readiness and peak CDR potentials over multiple decades [96].
- There is also a need to address the intangible aspects of NETs such as social acceptance, feasibility, secondary impacts, and co-benefits [30]. These aspects can be addressed by MCDA techniques. Models evaluating the synergistic and antagonistic effects between NETs are also needed. Portfolio optimization models can be used to determine the best mix of NETs considering these details.
- The data-driven approach in NETs planning is an emerging research area that is foreseen to grow in the future [9]. P-graph goes beyond supply chain synthesis by performing other tasks such as determining criteria weights using training data (similar to ML), generating optimal and suboptimal solutions for game theory, and producing causality maps. The use of P-graphs for NETs remains limited and presents an opportunity for further research.
- Lastly, planning NETs requires dealing with uncertainty [29]. Stochastic and robust MP models can be explored in future research.

The different techniques discussed in this work can be applied to the various tasks required in NETs planning to prescribe normative courses of action, rather than merely describing the results of predefined scenarios. These techniques can also mitigate the potential negative side impacts of NETs [17]. Planners need to carefully consider the local conditions before deploying NETs [1]. The optimization and decision support models presented in this work demonstrate the value of high-level decision support for developing climate policy.

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Author Contributions

Conceptualization: Raymond R. Tan.

Data curation: Maria Victoria Migo-Sumagang, Purusothmn Nair S. Bhasker Nair.

Formal analysis: Maria Victoria Migo-Sumagang, Kathleen B. Aviso.

Funding acquisition: Maria Victoria Migo-Sumagang, Dominic C. Y. Foo, Michael Short, Purusothmn Nair S. Bhasker Nair.

Methodology: Kathleen B. Aviso, Raymond R. Tan.

Project administration: Kathleen B. Aviso, Dominic C. Y. Foo, Michael Short.

Software: Maria Victoria Migo-Sumagang, Kathleen B. Aviso.

Supervision: Kathleen B. Aviso, Dominic C. Y. Foo, Michael Short, Raymond R. Tan.

Validation: Maria Victoria Migo-Sumagang, Kathleen B. Aviso.

Visualization: Maria Victoria Migo-Sumagang, Dominic C. Y. Foo, Michael Short, Purusothmn Nair S. Bhasker Nair.

Writing – original draft: Maria Victoria Migo-Sumagang.

Writing – review & editing: Kathleen B. Aviso, Dominic C. Y. Foo, Michael Short, Purusothmn Nair S. Bhasker Nair, Raymond R. Tan.

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