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Mathematical Modeling and Monte Carlo Simulation of Negative Emissions Technology Portfolios

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Negative emission technologies (NETs) support climate change mitigation by capturing carbon dioxide from the atmosphere for storage in a separate environmental compartment. NETs have multi-footprints that may negatively affect the environment and society if these technologies are implemented on large scales. The solution is implementing multiple technologies in NET portfolios at smaller scales for sustainability and risk reduction. However, computing optimal NET portfolios are challenged by uncertainties in the availability of resources that are difficult to predict precisely. This work implements a two-step approach to evaluating the robustness of NET portfolios. The first step is mathematical modeling to generate optimal and suboptimal solutions. The second step is subjecting the solutions to Monte Carlo simulation to evaluate the tradeoff between their cost and robustness against uncertain resource availability. The two-step approach is demonstrated in a case study on NET portfolios. Results show the existence of suboptimal solutions with higher costs but are more robust compared to the optimal solution. The two-step approach identifies the solutions that will perform well under uncertainty, thus supporting climate change mitigation decision analysis.

1. Introduction

The latest Intergovernmental Panel on Climate Change (IPCC) report declares that negative emission technologies (NETs) are now required to counterbalance the hard-to-abate emissions, especially in the energy sector (IPCC, 2022). NETs work by capturing carbon dioxide from the atmosphere and transferring it into the soil, biomass, construction materials, or in geological storage (Fuss et al., 2018). Examples of the prevalent land-based NETs from the literature include the biological options, afforestation/reforestation (AR), bioenergy with carbon capture and storage (BECCS), soil carbon sequestration (SCS), and biochar (BC); and the geochemical/chemical options, enhanced weathering (EW) and direct air carbon capture and storage (DACCS). NETs are characterized by multi-footprints such as land, water, energy, and nutrients that may impact the environment negatively when implemented on large scales (Smith et al., 2016). To sustainably deliver the required gigaton scale of negative emissions at lower risks, NET portfolios with the optimum technology mix are needed (Fuss et al., 2018). In portfolio optimization models, multi-footprints and resource limits must be considered to ensure sustainability (Čuček et al., 2012). However, the supply of resources is often uncertain due to variations in their availabilities. To address this challenge, computing techniques support the optimization of NET portfolios under uncertainties (Tan et al., 2022).

Currently, there are limited studies on NET portfolios and even fewer studies on evaluating the uncertainties in their deployment. A study employed post-optimization sensitivity analysis by varying the resource constraints in NET portfolios (Migo-Sumagang et al., 2021). Another study used fuzzy optimization to address both multi-objectivity and uncertainties in resource constraints (Migo-Sumagang et al., 2022). Neutrosophic data envelopment analysis, which addresses both risks and uncertainties, was developed and applied to NETs (Tapia, 2021). The mentioned approaches use deterministic models and evaluate the epistemic uncertainties or the uncertainties due to the lack of knowledge of the system. However, stochastic uncertainties due to parameter variations are also present in NETs optimization (Aviso et al., 2019). For example, the variations in the fertilizer and energy supply in small-scale applications should also be considered to ensure the continuous operation of these technologies.

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One approach is to generate optimal and suboptimal solutions during optimization, and then to further subject the solutions to Monte Carlo simulation (MCS) to check their robustness against parameter variations (Aviso et al., 2019). Since the optimal solution may be insufficient to address the problem as mathematical models do not represent the real world accurately, suboptimal solutions also need to be evaluated (Voll et al., 2015). The advantage of this approach is the identification of good solutions out of the suboptimal solutions that perform well despite the variations in the parameters (Aviso et al., 2019). This two-step approach has also been demonstrated in decarbonization portfolios, using process graphs (Tan et al., 2017) and mathematical modeling (Belmonte et al., 2020). So far, no studies have been found applying this two-step approach in NET portfolio modeling to assess the portfolios' robustness against the variations in resource availabilities. The benefit of applying this two-step approach to NET portfolios is the identification of solutions that are more robust compared to the optimal solution.

This work bridges the research gap by applying the two-step approach to NET portfolios. First, optimal and suboptimal solutions are generated through mathematical modeling. Next, the solutions are subjected to MCS, to test against varying resource availabilities. The second step identifies the solutions' probability of failure, which occurs when there is one or more violations in the constraints, in this case, when one or more resources becomes unavailable. A case study on optimal and suboptimal NET portfolios illustrates the technique. The main contribution of this study is modeling and evaluating robust NET portfolios, which support decision-making in climate change mitigation. The rest of the paper is organized as follows. Section 2 presents the problem statement. Section 3 discusses the methodology used. Section 4 shows an illustrative case study. And Section 5 gives the summary and conclusions of this work.

2. Problem statement

The formal problem can be stated as follows. Given a set of NETs $i \in I$ $(i = 1, 2, 3, \dots, N)$, and a set of resources $j \in J$ $(j = 1, 2, 3, \dots, R)$. Each resource j is characterized by its availability (F_j). Each NET i is characterized by its costs (C_i) and environmental footprints (M_{ij}) for each resource j. The problem is to find the optimum negative emissions allocation (x_i) of each NET i in a portfolio while minimizing the cost (C) and meeting the negative emissions target (G), resource constraints (F_j), upper (x_i^U), and lower (x_i^L) limits of NET potentials. It is also required to generate and select representative suboptimal solutions with configurations that are different from the optimal one. The performance of the optimal and representative suboptimal solutions against variations in resource availabilities is measured. The selection of the recommended portfolio is done after analyzing the performance of the optimal and representative suboptimal solutions.

3. Methodology

3.1 Optimization model

The model is represented by Eq(1) to Eq(6). The objective function, which minimizes the total cost of the portfolio, is shown in Eq(1), while the constraints are given by Eq(2) to Eq(6). The negative emissions target is shown in Eq(2), and the resource constraint based on the evaluation of the footprints is given in Eq(3). Since NETs have limited potential, they are constrained by Eq(4) and Eq(5). In this work, the lower limit (x_i^L) is assumed to be zero, which means a technology may be excluded from the portfolio. A binary variable (b_i) indicates whether a NET is selected $(b_i = 1)$ or not selected $(b_i = 0)$. The resulting model is a mixed integer linear programming (MILP) model, and the model is solved using an optimization software, LINGO 19.0 (LINDO, 2020).

$$\min \sum_i C_i x_i \tag{1}$$

$$\sum_i x_i \geq G \tag{2}$$

$$\sum_i M_{ij} x_i \leq F_j \quad , \forall j \tag{3}$$

$$x_i \geq b_i x_i^L \quad , \forall i \tag{4}$$

$$x_i \leq b_i x_i^U \quad , \forall i \tag{5}$$

$$b_i \in \{0,1\} \tag{6}$$

3.2 Generation of suboptimal solutions

After solving the model and generating the optimal solution, the suboptimal solutions are further generated using integer-cut constraints (Voll et al., 2015). The method is described as follows. In the known solutions $(\mathrm{k}-1)$, where i represents any solution, the binary variables $\mathrm{b}_{\mathrm{m}}^{(\mathrm{i})}$ represent the presence of stream m of the ith best solution. The streams are grouped into the sets, $\mathrm{M}_1^{(\mathrm{i})}$ and $\mathrm{M}_0^{(\mathrm{i})}$. The process streams in the ith best solution $\mathrm{b}_{\mathrm{m}}^{(\mathrm{i})}=1$ are depicted by $\mathrm{M}_1^{(\mathrm{i})}$ such that $\mathrm{M}_1^{(\mathrm{i})}=\left\{\mathrm{m}:\mathrm{b}_{\mathrm{m}}^{(\mathrm{i})}=1\right\}$, and the remaining streams $\mathrm{b}_{\mathrm{m}}^{(\mathrm{i})}=0$ are denoted by $\mathrm{M}_0^{(\mathrm{i})}$ such that $\mathrm{M}_0^{(\mathrm{i})}=\left\{\mathrm{m}:\mathrm{b}_{\mathrm{m}}^{(\mathrm{i})}=0\right\}$ (Voll et al., 2015).

The binary variables $\mathrm{b}_{\mathrm{m}}^{(\mathrm{k})}$ of the kth best solution in the $(\mathrm{k}-1)$ known solutions can be constrained by Eq(7), such that the inclusion of this constraint in the model makes the previous solution infeasible and the optimization generates the next best or kth best solution (Voll et al., 2015). This method is applied to generate suboptimal solutions. Representative suboptimal solutions with different configurations are selected for further analysis.

$$\sum\nolimits_{\mathrm{m}\epsilon\mathrm{M}_1^{(\mathrm{i})}}\left(\underbrace{b_{\mathrm{m}}^{(\mathrm{i})}}_{=1}-b_{\mathrm{m}}^{(\mathrm{k})}\right)+\sum\nolimits_{\mathrm{m}\epsilon\mathrm{M}_0^{(\mathrm{i})}}\left(\underbrace{b_{\mathrm{m}}^{(\mathrm{i})}}_{=0}-b_{\mathrm{m}}^{(\mathrm{k})}\right)\geq 1\ \forall\mathrm{i}\ \mathrm{i}=1,\ldots\mathrm{k}-1 \tag{7}$$

3.3 Monte Carlo simulation

The resulting optimal and suboptimal solutions are then subjected to MCS following the flowchart in Figure 1. Here, the model inputs refer to the resource constraints. First, the statistical properties of the model inputs, which are the probability distributions, are obtained. A random sample input is generated using the probability distribution of the model inputs. The sample input is used to calculate the model output in a simulation, and the result is recorded. The procedure is repeated until the number of iterations or simulations reaches a large number, in this case, 1,000. A network failure happens when one or more resource constraints are violated. The probability of failure $\mathrm{P(F)}$ is calculated by getting the percentage of the number of failed simulations divided by the total number of simulations specific to a resource. The overall $\mathrm{P(F)}$ is calculated by considering the failures in all the resources. The last step involves the analysis of the results, and the selection of the final solution for actual implementation based on the risk aversion of the decisionmaker.

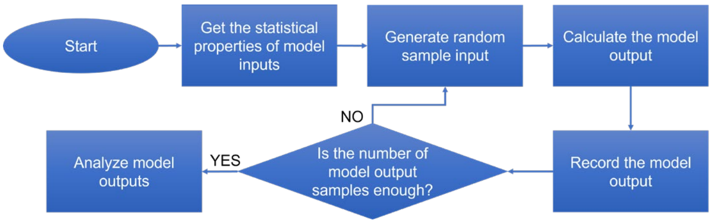

Figure 1: Monte Carlo Simulation (MCS) flowchart

4. Case study

The case study deals with an industry-scale application of a NET portfolio targeting a carbon dioxide removal of 50 Mt CO_2/y. The technology options consist of BECCS, AR, SCS, BC, DACCS, and EW. For this industry, it is assumed that the maximum potential of each NET is shown in Table 1. The data on the NET environmental footprints and costs are presented in Table 1 based on published literature as first used in the case study of Migo-Sumagang et al. (2022).

Table 1: NETs potential, environmental footprints, and cost

NET	Max potential (Mt CO_2/y)	Land (Mha/Gt CO_2)	Water (km³/Gt CO_2)	RE (EJ/Gt CO_2)	N (Mt/Gt CO_2)	P (Mt/Gt CO_2)	Cost (10^9 USD/Gt CO_2)
BECCS	15	114	574	0.605	9.57	6.65	150
AR	10	3	1575	0	0.11	0.13	27.5
SCS	10	0	0	0	22	5.5	50
BC	7.5	58	0	-35	8.2	2.7	75
DACCS	15	0.14	4.42	14.7	0	0	200
EW	20	85	1.5	6.4	0	0	125

Updated water footprints for BECCS and DACCS are used from a recent study (Rosa et al., 2021). It is assumed that the energy-consuming NETs would use renewable energy (RE), resulting in net negative emissions. The negative sign in the energy footprint of BC in Table 1 indicates energy production rather than consumption.
The mean and standard deviation values of the resource availabilities for this industry are found in Table 2. All the resources except for land are expected to have variations in their availability. It is assumed that the availabilities are normally distributed with a standard deviation equivalent to 15 % of the mean value for nitrogen and phosphorous (in the form of fertilizers), 5 % for water, and 20 % for RE due to higher fluctuations in supply and demand in RE for this industry. The standard deviations were estimated based on the annual consumption of the resources in the Philippines (The World Bank, 2022).

Table 2: Resource availability

Resource	Availability	Unit
Land	2.5	Mha/y
Water	20 ± 1	km^3/y
Renewable Energy (RE)	1.2 ± 0.24	EJ/y
Nitrogen (N)	0.3 ± 0.045	Mt/y
Phosphorous (P)	0.3 ± 0.045	Mt/y

Performing the model optimization and generation of suboptimal solutions in section 3 results in the optimal solution (rank 1) in Figure 2a and suboptimal solutions in Figures 2b to 2d, representing solution ranks 2, 4, and 5, respectively. Solution rank 3 was excluded from the selection as it has a similar configuration to solution rank 1 in terms of the selected NETs but varies according to the negative emissions allocation. All solutions achieved the negative emissions target of 50 Mt CO_2/y. Since the objective function minimizes the total cost of the portfolio, the suboptimal solutions expectedly result in higher costs. Each solution shows a different configuration with a different technology mix and different negative emission allocations for each NET (see Figure 2). Performing the MCS and calculating the probability of failure for each solution results in Table 3.

Table 3: MCS results for the optimal and selected suboptimal solutions

Solution	Total Cost (10^9 USD)	Probability of failure $\mathrm{P(F)}$ (%)				
		Water	Renewable Energy	Nitrogen	Phosphorous	Overall
Optimal (Rank 1)	4.25	0.2	0	48.4	0	48.5
Suboptimal						
Rank 2	4.34	0	0	36.4	0	36.4
Rank 4	5.28	0	0	3.7	0	3.7
Rank 5	5.69	0.2	0	0	0	0.2

Out of the four resources, the probability of failure is highest in nitrogen, indicating that this resource is the most binding. The probability of failure in water is minimal, while it is zero for renewable energy and phosphorous, indicating that these resources are more available for use in the NET portfolios. The optimal solution (rank 1) has an overall probability of failure equal to 48.5 %. In this solution, all six NETs are activated in the portfolio as shown in Figure 2a. Suboptimal solution rank 2 has a lower probability of failure (36.4 %) but is 2.1 % more costly than the optimal solution. Compared to the optimal solution, BECCS is deactivated and DACCS has a higher negative emissions allocation (2.5 Mt CO_2/y) in solution rank 2 (see Figure 2b). Suboptimal solution rank 4 has an even lower probability of failure (3.7 %) but is 24.2 % more costly than the optimal solution. In this solution, both BECCS and BC are deactivated in the portfolio, and the DACCS allocation is higher (10 Mt CO_2/y) (see Figure 2c). Lastly, the suboptimal solution rank 5 has the lowest probability of failure (0.2 %) but is 33.9 % more costly than the optimal solution. In this solution, SCS, which has the highest nitrogen requirement, is deactivated as shown in Figure 2d.
The results show that decreasing the allocation of the biologically based NETs, which require nitrogen, increases the robustness of the NET portfolio. However, this implies increasing the reliance on DACCS, which is currently the most expensive NET (USD 200/t CO_2). In all the solutions, EW and AR are consistently active and at their maximum potential. AR is the least costly NET (USD 27.5/t CO_2) and has the lowest nitrogen requirement among the biologically based NETs. EW, although one of the costliest NETs (USD 125/t CO_2), is less costly than DACCS and has zero nitrogen requirement.

The optimal and suboptimal solutions demonstrate the tradeoff between the cost and robustness of the solutions. Since the probability of failure depends on whether the solution is nitrogen-intensive, the decisionmaker may opt to find the "balance" between the nitrogen requirement of the solution while considering the impact on the cost. The decisionmaker may also consider the lowest probability of failure out of the representative solutions at the expense of a higher cost.

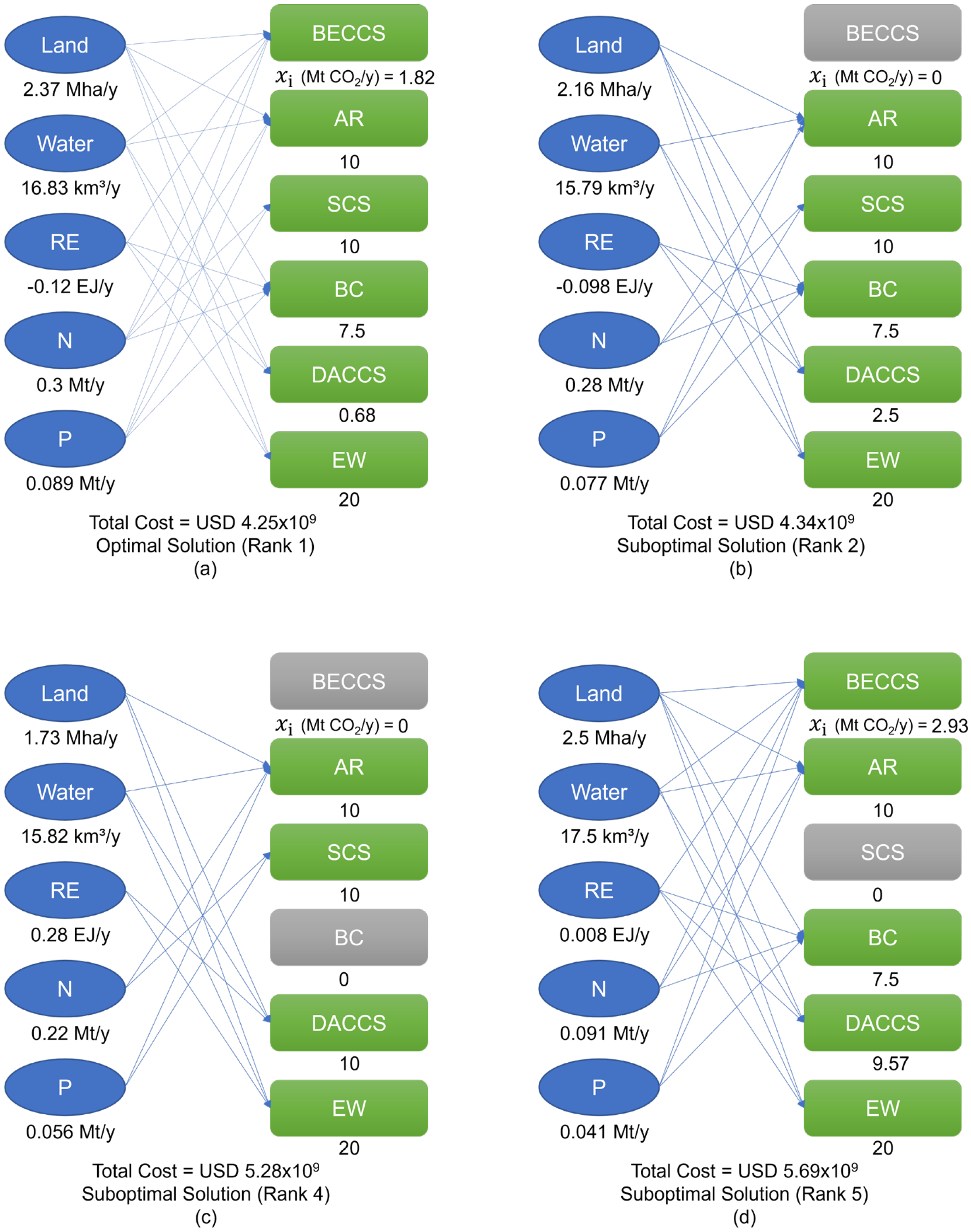

Figure 2: Optimal and suboptimal solutions. Active NETs, or NETs selected in the portfolio are indicated in green while inactive NETs are indicated in grey. The numbers below the NETs show the negative emissions allocation for each technology. The numbers below the resources show the total consumption for each resource.

5. Conclusions

This work implemented a two-step approach for generating and evaluating robust NET portfolios. The first step is mathematical modelling to generate optimal and suboptimal solutions. The second step is subjecting the solutions to MCS to evaluate their robustness under resource availability uncertainties. A case study using NETs reveals that the probability of failure of the solution is high depending on whether the solution is nitrogen-intensive. Suboptimal solutions that perform well under uncertainty but have a higher cost exist. The decisionmaker may opt to find a balanced solution with a low probability of failure and acceptable cost. This work supports the decision analysis in implementing NET portfolios for climate change mitigation. It is recommended to consider multi-periods that extend well beyond into the future since NETs must be implemented throughout the century. Other stochastic techniques may further elucidate the robustness of NET portfolios.

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