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Analysis of Optimum Negative Emissions Technology (NET) Portfolios Using Space-filling DOE Strategy

Maria Victoria Migo-Sumagang[a], Raymond R. Tan[b], Kathleen B. Aviso[b,*]

[a]Department of Chemical Engineering, University of the Philippines Los Baños, Laguna, Philippines
[b]Department of Chemical Engineering, De La Salle University, Manila, Philippines
kathleen.aviso@dlsu.edu.ph

Negative Emissions Technologies (NETs) are now necessary solutions for climate change mitigation. NET portfolios that recommend a technology mix of individual NETs at smaller scales are preferred to ease their implementation's environmental and social impact. Resource constraints using the Planetary Boundaries as a framework can be used to ensure that the multi-footprints of NETs are within the planet's safe operating space. However, for regional-scale applications, the uncertain resource constraints may highly depend on local conditions and the decisionmaker. There is a lack of studies investigating the effect of uncertain resource constraints on NET portfolios. This work addresses the research gap by applying a global sensitivity analysis using a space-filling Design of Experiments (DOE) strategy. First, a fuzzy, multi-period non-linear mathematical programming model is formulated. Computer experiments using a Latin hypercube space-filling DOE and regression analysis are then performed to investigate the effects of the varying resource constraints on the optimum NET portfolio. This approach enables the investigation of interactions and higher order effects of the parameters on the responses, the total negative emission potential and net present value of the portfolio, and the generation of response surface graphs, which are not available using traditional sensitivity analysis. The approach is demonstrated using a case study in the Association of Southeast Asian Nations region.

1. Introduction

Negative Emissions Technologies (NETs) sequester carbon dioxide from the atmosphere and include solutions such as Afforestation/Reforestation (AR), BioChar (BC) application, Soil Carbon Sequestration (SCS), Bioenergy with Carbon Capture and Storage (BECCS), Enhanced Weathering (EW), and Direct Air Carbon Capture and Storage (DACCS). Based on the latest Intergovernmental Panel on Climate Change (IPCC) report, NETs have become part of the portfolio of solutions against climate change to counter residual emissions from the hard-to-abate sectors (IPCC, 2022). The large-scale implementations of NETs have environmental footprints that may negatively impact the environment and society; thus, it is recommended to implement portfolio solutions of individual NETs at reduced scales (Tan et al., 2022). The Planetary Boundaries (Rockström et al., 2009) serve as a framework for evaluating the resource constraints of NETs. For regional scales, the resource constraints can be estimated by scaling down the Planetary Boundaries but are still highly dependent on local conditions and the decisionmaker. Hence, there is a strong need to investigate the effect of resource constraints on the corresponding optimum NET portfolio.
Traditional sensitivity analysis in optimization software uses dual prices for linear models and Lagrange multipliers for non-linear models (Tan et al., 2015). For non-linear models, Lagrange multipliers are restricted since they only investigate the changes in the optimal value of the objective function with respect to small changes in the parameters, and they fail to investigate the combined effects of simultaneous changes in the parameters (Tan et al., 2015). To address these limitations, a study proposed the use of the space-filling Design of Experiments (DOE), particularly the Latin Hypercube Design (LHD), as a global sensitivity analysis (Tan et al., 2015). Ibrahim et al. (2009) also proposed using a small design, such as LHD or Sobol sequence and an ANOVA-type decomposition to assess the higher-order effects. The LHD, as DOE, has an advantage because of its simplicity and ease of generation of the designs (Ibrahim et al., 2009).

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Only a very limited number of studies have investigated the effect of varying resource constraints on NET portfolios. Migo-Sumagang et al. (2021) performed a sensitivity analysis on a linear programming model for optimizing NET portfolios by varying the resource constraints one parameter at a time. The limitation of this approach is that the interaction and higher-order effects are not captured in the analysis. Analyzing these effects on resource constraints evaluation is important because they show which resources have interactions. When an interaction between parameters exists, the effect of one parameter depends on the value of the other parameter; but when there is no interaction, the effect of these parameters is simply additive (Ibrahim et al., 2009). Another study developed a fuzzy mathematical programming model to optimize NET portfolios under fuzzy resource constraints and used the dual price value reported by the optimization software for the sensitivity analysis (Migo-Sumagang et al., 2022). However, this approach has the same limitations as the previous study. There is an overall lack of studies investigating the effect of varying resource constraints on NET portfolios.
To address this research gap, this work first develops a novel fuzzy mixed-integer non-linear programming (MINLP) model to optimize a NET portfolio under multi-footprint and multi-period constraints. Next, a global sensitivity analysis is performed on the optimization model through computer experiments using the space-filling LHD and subsequent regression analysis. The rest of the paper is organized as follows. Section 2 discusses the methodology performed in this work. Section 3 presents a case study on the Association of Southeast Asian Nations (ASEAN) region. And section 4 summarizes and concludes the main points of this study.

2. Methodology

This section describes the problem statement, optimization model, and the methodology based on space-filling DOE.

2.1 Formal problem statement

The problem is formally stated as follows. Given a set of resources. Each resource j is characterized by its fuzzy resource constraint (F_{jk}) for each period k, defined in the interval (F_{jk}^{L}, F_{jk}^{U}). Given a set of NETs. Each net i is characterized by its fuzzy environmental footprints (M_{ijk}) for each resource j and for each period k, defined in the interval (M_{ijk}^{L}, M_{ijk}^{U}). Given the upper (x_{ik}^{U}) and lower (x_{ik}^{L}) annual NET capacities, cumulative capacity (S_i), and costs (C_{ik}) of NETs for each period k. NETs using geological storage are given a fuzzy cumulative geological storage limit defined in the interval (Q^{L}, Q^{U}). Given the possible synergistic interactions between NETs, two synergistic NETs are subject to a resource discount rate (α_{ilj}) when implemented together in the portfolio. Given a carbon price (P_k) for each period. The cost of NET and the carbon price are subject to an economic discount rate (r_E). The aim of the problem is to determine the optimum negative emission allocation (x_{ik}) of each NET in each period while maximizing both the fuzzy net present value (NPV) of the NET portfolio defined in the interval (V^{L}, V^{U}), and the fuzzy negative emission potential (G) defined in the interval (G^{L}, G^{U}) while meeting the resource and capacity constraints. The planning horizon consists of time intervals given by ΔK.

2.2 Optimization model

The fuzzy optimization model based on the formulation of (Zimmermann, 1978) is depicted in Eq(1) to (16). The objective function maximizes the overall degree of satisfaction (λ) in Eq(1), where λ is restricted between 0 and 1. The fuzzy constraint in Eq(3) aims to maximize the NPV of the portfolio subject to the discount rate (r_E). As λ is maximized and approaches the value 1, the right term of Eq(3) approaches the upper limit of the NPV (V^{U}) as opposed to the lower limit (V^{L}). Similarly, Eq(4) maximizes the negative emission potential (G) of the portfolio since the right term approaches the upper limit (G^{U}) as opposed to the lower limit (G^{L}) as λ approaches the value 1. Eq(5) introduces a binary variable (b_{ik}) and ensures that the negative emission allocation (x_{ik}) of each NET in each period k is within than the upper (x_{ik}^{U}) and lower (x_{ik}^{L}) capacity limits. Eq(6) is the cumulative NET capacity constraint (S_i). Eq(7) is the fuzzy cumulative geological storage capacity constraint (Q) for NETs with geological storage. The topological parameter (z_i) is assigned a value of 1 for NETs with geological storage; otherwise, it is set to 0. The right-hand side of Eq(7) approaches the lower limit of the geological storage (Q^{L}) as λ approaches the value 1, which is preferred by a conservative decisionmaker. Eqs(8) to (10) introduce another binary variable (int_{ilk}), which activates and takes the value of 1 when two NETs i and l are present simultaneously in the portfolio, based on the formulation by Weber et al. (1990). This variable will be used in the evaluation of any synergistic resource interactions between NETs. Eq(11) is the resource constraint with an evaluation of synergistic resource interactions. The left side of Eq(11) evaluates the fuzzy NET environmental footprints (M_{ijk}), which must be less than the fuzzy resource constraint (F_{jk}). The second term on the right side of Eq(11) is the synergistic resource interaction term, which activates when both the resource discount rate (α_{ilj}) and binary variable int_{ilk} are non-zero. Eq(12) and (13) are the fuzzy constraints for the resource limit (F_{jk}) and environmental footprint (M_{ijk}), which are minimized and maximized, respectively, following the preference of a conservative decisionmaker. Eq(14) is a special case for synergistic land interaction, which allows NETs to be implemented on the same land simultaneously (Migo-Sumagang et al., 2022). Eq(15) ensures that once a NET is activated, it will remain activated in the portfolio throughout the rest of the planning horizon. The model described here is a mixed integer non-linear programming (MINLP) model.

$$\max \lambda \quad (1)$$

$$0 \leq \lambda \leq 1 \quad (2)$$

$$\sum_i \sum_k x_{ik}(P_k - C_{ik})\left(\left(\frac{(1+r_E)^{\Delta K}-1}{r_E}\right)(1+r_E)^{-\Delta Kk}\right) \geq V^L + \lambda(V^U - V^L) \quad (3)$$

$$\sum_i \sum_k x_{ik}\Delta K \geq G^L + \lambda(G^U - G^L) \quad (4)$$

$$b_{ik}x_{ik}^L \leq x_{ik} \leq b_{ik}x_{ik}^U \ , \forall i,k \quad (5)$$

$$\sum_k x_{ik}\Delta K \leq S_i \ , \forall i \quad (6)$$

$$\sum_i \sum_k x_{ik}z_i\Delta K \leq Q^U + \lambda(Q^L - Q^U) \quad (7)$$

$$b_{ik} \geq int_{ilk} \ , \forall i,l,k \quad (8)$$

$$b_{lk} \geq int_{ilk} \ , \forall i,l,k \quad (9)$$

$$b_{ik} + b_{lk} - 1 \leq int_{ilk} \ , \forall i,l,k \quad (10)$$

$$\sum_i x_{ik}M_{ijk} \leq F_{jk} + \sum_i \sum_l \alpha_{ilj} int_{ilk} x_{ik} M_{ijk} \ , \ \forall j,k \quad (11)$$

$$F_{jk} \leq F_{jk}^U + \lambda\left(F_{jk}^L - F_{jk}^U\right), \forall j,k \quad (12)$$

$$M_{ijk} \geq M_{ijk}^L + \lambda\left(M_{ijk}^U - M_{ijk}^L\right) \ , \ \forall i,j,k \quad (13)$$

$$\beta_i x_{ik} M_{ijk} + \sum_l (1-\beta_l) x_{il} M_{ijk} \leq F_{jk} \ , \ \forall i,k \quad (14)$$

$$b_{ik} \leq b_{i(k+1)} \ , \forall i,k,k+1 \quad (15)$$

$$b_{ik}, b_{lk}, int_{ilk} \in \{0,1\} \quad (16)$$

2.3 Sensitivity analysis using a space-filling DOE

The following procedure is based on the study by (Tan et al., 2015), using the LHD sampling technique, first described by McKay et al. (1979).

- Given an optimization model. Its objective function is defined by $f(x)$ where x is the decision variable. The optimal solution of the objective function is given by $f(x^*)$.
- The model has uncertain parameters (b) limited by upper (b_U) and lower (b_L) bounds, thus defining the factor space. A unique optimal solution can be derived for each point within the factor space.
- A space-filling design, LHD, is used as a sampling technique in the factor space. Sufficient points are sampled to satisfy the degrees of freedom for statistical analysis.
- The model is evaluated for each point in the design.
- Regression analysis is done on the solutions, giving a statistically significant polynomial regression model that closely approximates the true response surface of the MINLP to parameter variations. This derived model serves as an estimate of the optimal solution $f(x^*)$ as a function of the uncertain parameters (b).

The procedure is implemented on the MINLP optimization model described in the previous subsection. The optimization model is solved using LINGO 19.0 by Lindo Systems, which uses the branch and bound algorithm solver for non-linear models (Gau and Schrage, 2004). The generation of the LHD (McKay et al., 1979), statistical analysis, and generation of the response surfaces are done using the software Stat-Ease 360 by Stat-Ease.

3. Case study

The case study investigates the optimal NET portfolio in the ASEAN region throughout the end of the 21st century. Six terrestrial NETs, AR, BECCS, DACCS, SCS, BC, and EW, are included in the study. The data on the fuzzy NET environmental footprints (M_{ijk}), regional NET capacities (x_{ik}^{L} and x_{ik}^{U}), and the fuzzy negative emissions target (G^{L} and G^{U}) are obtained from various references as first gathered by Migo-Sumagang et al. (2022). The fuzzy geological storage limit is 49.7 (Q^{L}) to 54 (Q^{U}) Gt CO_2 (Asian Development Bank, 2013). The planning horizon is from 2020 to 2100, divided into eight periods with a time interval of $\Delta K = 10$ years. This corresponds to a cumulative negative emissions target projection equal to 30 (G^{L}) to 58 (G^{U}) Gt CO_2 for the region (Migo-Sumagang et al., 2022). Future projections of carbon prices (Strefler et al., 2021) and NET costs (Fuss et al., 2018) are used, as first seen in the case study of Migo-Sumagang et al. (2023). For BECCS, DACCS, and EW, cost projections are based on land competition and technology improvements (Creutzig et al., 2019), while for AR, SCS, and BC, costs are assumed to be stable. The future regional NET capacities are based on scaled-down global NET capacities (Rueda et al., 2021) as in the case study of Migo-Sumagang et al. (2023). It is assumed that EW and BC have land and cost synergistic interaction ($\alpha_{ilj} = 10$ %) since the two NETs can be applied on the same land and can share supply chains. An economic discount rate equal to 3 % is used, which is the central value used in literature (U.S. IAWG, 2021). The fuzzy upper limits (F_{jk}^{U}) of the resource constraints in 2020 are 45.70 Mha for land, 1135 km^3 for water, 19.50 EJ for energy, and 6.2 Mt for both nitrogen and phosphorous (Migo-Sumagang et al., 2022). These initial values are projected into the future using GDP calculations, assuming limited resources for land, water, nitrogen, and phosphorous; and a stable and steady supply of renewable energy (Migo-Sumagang et al., 2023). On the other hand, the fuzzy lower limits (F_{jk}^{L}) are set to zero for minimization purposes.

The sensitivity analysis following the procedure in section 2.3 evaluates the uncertain upper limits in the resource constraints. For the computer experiments, the upper bounds are set to equal to the fuzzy upper limits (F_{jk}^{U}) while the lower bounds are assumed to be half of these values. Note that setting the lower bounds to zero in the computer experiments potentially results in infeasible solutions. For simplicity, nitrogen and phosphorous are considered as one factor (as nutrients) as they have the same upper bound. Four factors, land (A), water (B), energy (C), and nutrients (D), and two responses, the negative emission potential (G) and NPV, are considered in the computer experiments. The generated LHD has 16 design points and can detect linear, two-factor interaction, and quadratic effects. The fit summary is checked during the statistical analysis. The F-value tests the significance of adding linear, two-factor interaction, and quadratic terms to the regression model (State-Ease, 2021). A small p-value (Prob > F) indicates that adding these terms has improved the regression model (State-Ease, 2021). Table 1 summarizes the statistical analysis of the regression model for the response G, and Table 2 summarizes the analysis of the response NPV. Terms with a p-value less than 0.05 indicate a statistically significant signal, while the signs indicate the direction of the effect.

For response G, the resulting regression model is linear since the quadratic effects (A^2, B^2, C^2, D^2) are insignificant. The response surface graph of land (A) and water (B) in Figure 1a shows the linear relationship of the two parameters on the response. Only the individual effects of three terms (A, B, and D) are found to be statistically significant, with a positive effect on the response. A positive effect is expected since increasing the resource limits would increase G. It is possible that energy is not found to be statistically significant on response G due to the binding effect of the other resources within the bounds considered. The interaction terms (AB, AC, AD, BC, BD) are not found significant, indicating that the effects of the parameters on G are additive.

For response NPV, all three terms (A, B, and D), the interaction between land and water (AB) and between land and nutrients (AD), and the quadratic terms for land (B^2) and energy (C^2) are found to be significant. The linear effect of energy is insignificant, but due to hierarchy, it is included in the model. Negative interaction effects indicate that the combined effect of the two factors is less than the sum of their individual effects. This means the combined effect of land with water (AB) or the nutrients (AD) do not increase or equal the sum of their individual effects on the NPV. The response surface graphs of the combined effects are shown in Figures 1b and 1a. Quadratic effects indicate a non-linear relationship, which is true for water (B^2) and energy (C^2). The negative quadratic effect of water (- 5.52) indicates that for low values of the parameter, the effect on the NPV is positive, but for higher values, the effect becomes negative. On the other hand, the positive quadratic effect of energy on NPV (+ 1.25) suggests that the relationship is exponential. Overall, the region with the highest degree of satisfaction considering both G and NPV is the region with warm colors in the response surface graphs (see Figure 1).

Table 1: Effect of model parameters on the negative emission potential (G)

Term	Estimate	p-value	Remark
C, AB, AC, AD, BC, BD, CD, A^2, B^2, C^2, D^2	0*	> 0.05	Not statistically significant
A	+ 0.4671	0.0118	Statistically significant positive effect
B	+ 0.9607	< 0.0001	Statistically significant positive effect
D	+ 0.3954	0.0270	Statistically significant positive effect

Table 2: Effect of model parameters on the NPV

Term	Estimate	p-value	Remark
AC, BC, BD, CD, A^2, D^2	0*	> 0.05	Not statistically significant
A	+ 26.91	< 0.0001	Statistically significant positive effect
B	+ 42.25	< 0.0001	Statistically significant positive effect
C	- 0.065	0.7913	Not statistically significant
D	+ 25.52	< 0.0001	Statistically significant positive effect
AB	- 2	0.0034	Statistically significant negative effect
AD	- 2.53	0.0012	Statistically significant negative effect
B^2	- 5.52	< 0.0001	Statistically significant negative effect
C^2	+ 1.25	0.0271	Statistically significant positive effect

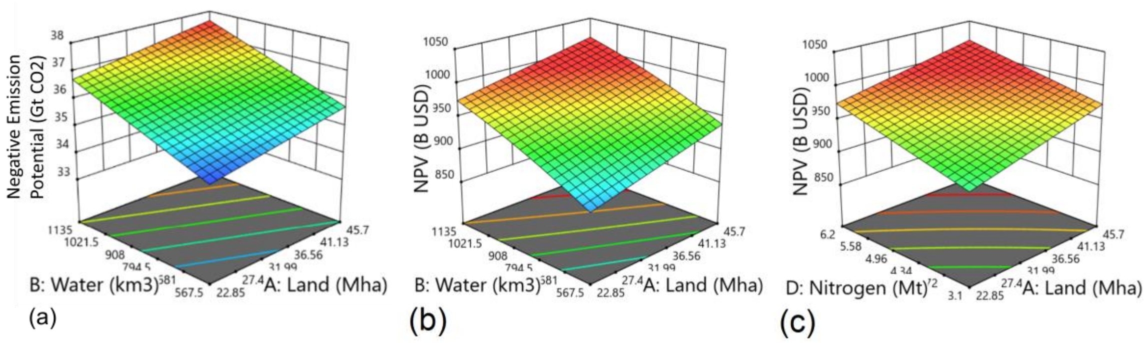

Figure 1: Response surface graphs of land and water on G (a) and NPV (b); and land and nutrients on the NPV

4. Conclusions

A fuzzy multi-period MINLP model for NET portfolio optimization has been developed and subjected to global sensitivity analysis using a space-filling DOE. The approach has an advantage over the Lagrange multipliers being used by commercial software for the sensitivity analysis of non-linear models since the latter is limited to investigating only small changes in the optimal value of the objective function with respect to small changes in the parameters. The space-filling DOE sensitivity analysis also has an advantage over the traditional sensitivity analysis because it evaluates the combined effects of the parameters. To illustrate the approach, the case study shows a linear effect of land, water, and nutrients on the total negative emission potential of the portfolio and the linear, interaction, and quadratic effects of the parameters on the NPV. The case study demonstrates the detection of interaction and quadratic effects and the generation of response surface graphs, which are not available in a traditional sensitivity analysis. Future work can investigate the effect of other factors on the responses.

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References

Asian Development Bank, 2013, Prospects for Carbon Capture and Storage in Southeast Asia, Asian Development Bank, Manila, Philippines.

Creutzig F., Breyer C., Hilaire J., Minx J., Peters G.P., Socolow R., 2019, The mutual dependence of negative emission technologies and energy systems, Energy and Environmental Science, 12, 1805–1817.
Fuss S., Lamb W.F., Callaghan M.W., Hilaire J., Creutzig F., Amann T., Beringer T., De Oliveira Garcia W., Hartmann J., Khanna, T., Luderer G., Nemet G.F., Rogelj J., Smith P., Vicente J.V., Wilcox J., Del Mar Zamora Dominguez M., Minx J.C., 2018, Negative emissions - Part 2: Costs, potentials and side effects, Environmental Research Letters, 13, 063002.
Gau C.-Y., Schrage L.E., 2004, Implementation and Testing of a Branch-and-Bound Based Method for Deterministic Global Optimization: Operations Research Applications. In: Floudas, C.., Pardalos, P. (Eds.), Frontiers in Global Optimization, Nonconvex Optimization and Its Applications, Springer, Boston, MA, Boston, pp. 145–164.
Ibrahim J., Chen M.-H., Sinha D., 2009, The Design and Analysis of Computer Experiments, Springer Series in Statistics, New York, USA.
IPCC 2022, Mitigation of Climate Change (Summary for Policymakers), Cambridge University Press, Cambridge, UK and New York, NY, USA.
McKay M.D., Beckman R.J., Conover W.J., 1979, A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output from a Computer Code, Technometrics, 21, 239.
Migo-Sumagang M.V., Aviso K., Tapia J.F., Tan R.R., 2021, A Superstructure Model for Integrated Deployment of Negative Emissions Technologies under Resource Constraints, Chemical Engineering Transactions, 88, 31–36.
Migo-Sumagang M.V., Tan R.R., Tapia J.F.D., Aviso K.B., 2022, Fuzzy mixed-integer linear and quadratic programming models for planning negative emissions technologies portfolios with synergistic interactions, Cleaner Engineering and Technology, 9, 100507.
Migo-Sumagang M.V., Tan R.R., Aviso K.B., 2023, A multi-period model for optimizing negative emission technology portfolios with economic and carbon value discount rates, Energy, 127445.
Rockström J., Steffen W., Noone K., Persson Å., III, F.S.C., Lambin E.F., Lenton T.M., Scheffer M., Folke C., Schellnhuber H.J., Nykvist B., Wit C.A. de, Hughes T., Leeuw S. van der, Rodhe H., Sörlin S., Snyder P.K., Costanza R., Svedin U., Falkenmark M., Karlberg L., Corell R.W., Fabry V.J., Hansen J., Walker B., Liverman D., Richardson K., Crutzen P., Foley J.A., 2009, A safe operating space for humanity, Nature, 461, 472–475.
Rueda O., Mogollón J.M., Tukker A., Scherer L., 2021, Negative-emissions technology portfolios to meet the 1.5 °C target, Global Environmental Change, 67, 102238.
Stat-Ease 2021, Fit Summary (RSM/MIX Model Selection), Design Expert Inc. <www.statease.com/docs/v11/contents/analysis/fit-summary/>, accessed 11.04.2023.
Strefler J., Kriegler E., Bauer N., Luderer G., Pietzcker R.C., Giannousakis A., Edenhofer O., 2021, Alternative carbon price trajectories can avoid excessive carbon removal, Nature Communications, 12, 2264.
Tan R.R., Aviso K.B., Foo D.C.Y., Migo-sumagang M.V., Nair P., Nair S.B., Short M., 2022, Computing optimal carbon dioxide removal portfolios, Nature Computational Science, 2, 465–466.
Tan R.R., Aviso K.B., Uy O.M., 2015, Comprehensive sensitivity analysis in NLP models in PSE applications using space-filling DOE strategy, Chemical Engineering Transactions, 45, 523–528.
U.S. IAWG, 2021, Technical support document: Social cost of carbon, methane, and nitrous oxide, Interagency Working Group on Social Cost of Greenhouse Gases, Washington, USA.
Weber R., Werners B., Zimmermann H.J., 1990, Planning models for research and development, European Journal of Operational Research, 48, 175–188.
Zimmermann H.J., 1978, Fuzzy programming and linear programming with several objective functions, Fuzzy Sets and Systems, 1, 45–55.