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A Superstructure Model for Integrated Deployment of Negative Emissions Technologies under Resource Constraints

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Negative Emissions Technologies (NETs) will be needed in order to achieve the net zero emissions targets being set by many countries. These technologies will offset the residual greenhouse gas emissions of sectors that are inherently difficult to decarbonize. NETs draw down carbon through different physical, chemical, or biological pathways, and transfer it for storage to other environmental compartments. Examples of these techniques include afforestation, Biochar application, BioEnergy with Carbon Capture and Storage (BECCS), enhanced weathering, and Direct Air Capture (DAC). The large-scale deployment of NETs will be constrained by the footprints they apply to limited resources such as land, water, energy, and nutrients. In this work, a superstructure-based Linear Programming (LP) model is developed to optimize the carbon drawdown of integrated NET deployment under resource constraints. Results show that varying the target negative emissions and resource constraints affect the NETs portfolio and total cost.

1. Introduction

Global efforts are now focused on climate change mitigation as nations have reached a consensus during the Paris Agreement in 2015 to keep global warming "well below" 2 °C (Hilaire et al., 2019). Several countries have signified their ambitious goal of net zero emissions by 2050 at the UN Climate Change Conference in 2019 (Gani, 2021). To increase the chances of achieving the below 2 °C target and to reach net zero emissions, integrated assessment models show that Negative Emission Technologies (NETs) are necessary (Smith et al., 2016a). NETs remove carbon from the atmosphere via physical, chemical, or biological pathways, so that the resulting atmospheric concentrations are lower before their deployment (McLaren, 2012). NETs can be implemented terrestrially, such as in BioEnergy with Carbon Capture and Storage (BECCS), Afforestation and Reforestation (AR), Biochar, Soil Carbon Sequestration (SCS), Direct Air Capture (DAC), and Enhanced Weathering (EW) (Smith et al., 2016b). The exact amount of carbon removal required of NETs in the next decades is highly dependent on the decarbonization of different sectors. However, the Fifth Assessment Report by the Intergovernmental Panel on Climate Change emphasized that NETs deployment by 2050 will play a big role in achieving the targets, since immediate decarbonization of some sectors is not possible (Hilaire et al., 2019).

With the rising popularity of NETs, the negative emission capacities, technology readiness, and cost of NETs have been assessed in various literature. Among the NETs, DAC is seen to have the highest potential, reaching over a removal rate of 2.73 Gt C eq./y, while BECCS runs second having a potential of 0.55 to 2.73 Gt C eq./y (McLaren, 2012). The rest of the NETs range from 0.27 to 0.82 Gt C eq./y (McLaren, 2012). As with the large-scale implementation of new technologies, concerns on the feasibility and sustainability are being raised. Smith et al. (2016b) investigated the impact of NETs on different resources per unit of negative emissions. BECCS has a land use intensity ranging from 0.1 to 1.7 ha·y/t C eq., depending on the feedstock used, while DAC and EW have a land use intensity of less than 0.01 ha·y/t C eq. DAC and EW require very high energy input of about 45 to 46 GJ/t C eq., while BECCS produces an energy output of 3 to 40 GJ/t C eq. NETs relying on biomass

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(BECCS, Biochar, and AR) have nitrogen, phosphorous, and water footprints (Čuček et al., 2012) while DAC and EW have relatively insignificant values for these footprints. Since NETs have varying impacts on resources, it is crucial to consider sustainable development when choosing a portfolio of NETs.

Mathematical programming is a powerful Process Integration (PI) tool for the large-scale implementation of technologies (Klemeš, 2013). For example, a linear program (LP) was used in optimizing EW networks, via a source-sink model (Tan and Aviso, 2019). Ng et al. (2020) ranked NETs under uncertainty considering technical status, potential capacity, cost, and energy requirement using non-linear programming. An approach using superstructure-based optimization, which embeds many alternative matches, covering all possible interconnections that are candidates for the optimal design (Smith, 2016) can serve as a powerful tool in integrated NET deployment. The superstructure approach has various applications such as in Heat Exchanger Network (HEN) synthesis (Beck and Hofmann, 2018) and planning of carbon capture, utilization, and storage (CCUS) systems (Zhang et al., 2020). To date, no studies have been found on superstructure-based optimization models of NETs under resource constraints using the search keywords "negative emission technology" and "superstructure" and "optimization" in the Scopus database.

To address this research gap, this paper develops a generic superstructure-based LP model for the integrated deployment of NETs, taking into account resource constraints. The rest of the paper is organized as follows. Section 2 gives the problem statement. Section 3 presents the optimization model. Section 4 illustrates a case study using literature data from the UK. Section 5 presents the sensitivity analysis of the model. Lastly, section 6 gives the conclusions of this paper.

2. Problem statement

Given a set of negative emission technologies (NET), and a set of resources (land, water, energy, etc.). Each NET is characterized by its impact on the resources per unit of negative emissions. The problem is to find the optimal amount of negative emissions allocation for each NET to optimize the cost while achieving a negative emissions target and satisfying the resource constraints for sustainability. The model will give the optimal portfolio of NETs and their recommended capacities while ensuring that the selected NETs perform under the given resource limits. Figure 1 shows the superstructure of the proposed model.



Figure 1: Superstructure model for the integrated deployment of NETs

3. Optimization model

The LP model is:	
min $\sum_i C_i x_i$	(1)
subject to:	
$\sum_i x_i \ge GT$	(2)

$$\sum_{i} x_{i} M_{ij} \leq F_{j}$$
 , $\forall j$

where x_i is the negative emissions allocation for each NET i, C_i is the economic cost factor of each NET i per unit of negative emissions, GT is the negative emissions target, M_{ij} is the individual impact of each NET i on each resource j per unit of negative emissions, and F_i is the selected limits of each resource j.

(3)

Eq(1) aims to minimize a linear cost function of the negative emissions allocation. The first constraint, Eq(2), ensures that the negative emissions target (GT) is achieved. Eq(3) ensures that the impacts on each resource j (land use, water use, etc.) are within the selected limits. It was assumed that land use among NETs is mutually

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exclusive, although the effect of some NETs on land use can be additive (Smith et al., 2019). The permanence and sink saturation of some NETs (SCS, AR, and Biochar) (Smith et al., 2016a) are not covered in this model.

4. Case study

Six terrestrial NETs are considered, namely, BECCS, AR, SCS, Biochar, DAC, and EW. The impacts of each NET on a per t C eq. negative emissions are found in Table 1, using the low-values scenario in the UK (Smith et al., 2016a). It is useful to note that some impacts are zero or relatively insignificant compared to the other NETs, such as the water use of SCS and Biochar, energy input of AR and SCS, and the nutrient requirements of DAC and EW. Also, the energy inputs of BECCS and Biochar are negative, which means these NETs generate rather than consume energy. The costs of SCS and Biochar are also negative, indicating cost savings.

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NET	Land use	Water use	Energy input	Nitrogen	Phosphorus	Cost
	(ha/t C eq.)	(k(m ³)/t C eq.)	(GJ/t C eq.)	(kg/t C eq.)	(kg/t C eq.)	(USD/t C eq.)
BECCS	0.1	2	-38.6	11	0.8	132
AR	0.1	1.8	0	2	4	65
SCS	1	0	0	80	20	–165
Biochar	0.13	0	-50	30	10	-830
DAC	0.001	0.073	2.6	0	0	1,600
EW	1.22	0.0015	3	0	0	92

Table 1: Impacts and cost of NETs on a per t C eq. negative emissions (Smith et al., 2016a)

The target negative emission is based on removal rates of 2.18 to 6.54 Gt C eq./y to achieve 350 ppm (McLaren, 2012). As discussed, the actual target depends on many factors such as energy decarbonization timelines. A stringent scenario of 6.54 Gt C eq./y is selected for this case study. Global land use limit is based on the difference between the proposed limit of land cover converted to cropland (15 %) and the 2009 status (11.7 %) (Rockström et al., 2009). The difference (3.3 %) is multiplied with the global land area (13.2 Gha) to find the land area limit (436 Mha). The global freshwater supply limit is assumed to be 1,400 km³/y, based on the difference between the proposed global limit (4,000 km³/y) and the 2009 global freshwater use (2,600 km³/y) (Rockström et al., 2009).

The available bioenergy supply in 2050 is 10 to 245 EJ/y based on Integrated Assessment Models (Smith et al., 2016b). A scenario where NETs are self-sustaining is selected; the energy supply limit is assumed to be 10 EJ/y. The proposed boundary for nitrogen removed from the atmosphere is 35 Mt/y but the current status is above this value, at 121 Mt/y (Rockström et al., 2009). Capping the nitrogen footprint to zero will limit the options to DAC or EW based on their nitrogen impacts (0 kg N/C eq.). A scenario where the nitrogen limit is set to 3.5 Mt/y (10 % of the proposed boundary) is investigated. On the other hand, the phosphorous limit is set to 1.5 Mt/y based on the difference between the proposed boundary (11 Mt/y) and the current status (8.5-9.5 Mt/y) (Rockström et al., 2009). It was assumed that the availability of suitable rock for EW is not limiting since the order of magnitude of alkaline minerals far exceeds CDR requirements (Smith et al., 2016b). The summary of the selected resource constraints is in Table 2.

Table 2: Selected resource constraints

Resource	Limit	Source
Land use (Mha)	436	(Rockström et al., 2009)
Water use (km ³ /y)	1,400	(Rockström et al., 2009)
Energy input (EJ/y)	10	(Smith et al., 2016a)
Nitrogen (Mt/y)	3.5	(Rockström et al., 2009)
Phosphorous (Mt/y)	1.5	(Rockström et al., 2009)
Suitable rock for EW	unlimited	(Smith et al., 2016b)

Solving Eq(1) subject to constraints in Eq(2) and Eq(3) results in an optimal NETs portfolio found in Table 3. The model only selects the combination of BECCS, Biochar, DAC, and EW, and leaves out AR and SCS in the profile to achieve the negative emissions target (6.54 Gt C eq./y). Among the NETs selected, EW has the highest (4.58 Gt C eq./y) while Biochar has the lowest (0.07 Gt C eq./y) allocated capacity in the negative emissions. All the resource constraints are maximized except for water use and phosphorous requirement, which are below their respective limits. The total cost to achieve this scenario is USD 3,195.67 x 10^9 /y.

NET	Negative Emissions (Gt C eq./y)	Land Use (Mha)	Water use (km ³ /y)	Energy input (EJ/y)	Nitrogen (Mt N/y)	Phosphorus (Mt P/y)	Cost (10 ⁹ USD/y)
BECCS	0.12	12.33	246.54	-4.76	1.36	0.10	16.27
AR	0	0	0	0	0	0	0
SCS	0	0	0	0	0	0	0
Biochar	0.07	9.29	0.00	-3.57	2.14	0.71	-59.32
DAC	1.76	0	128.52	4.58	0.00	0.00	2,816.92
EW	4.58	412.62	6.88	13.75	0.00	0.00	421.79
Total	6.54	436.00	381.93	10.00	3.50	0.81	3,195.67

Table 3: Optimal NET portfolio at a negative emission target of 6.54 Gt C eq./y and specified resource constraints

5. Sensitivity analysis

The effect of varying negative emissions target on the resources and total cost, as well as the effect of varying resource constraints on the total cost were investigated in this section.

5.1 Effect of varying negative emissions target

The negative emissions target was varied in the range 2.18 to 6.54 Gt C eq./y (McLaren, 2012). The range was divided into 10 increments, and each step was used as the negative emissions target while keeping the resource limits in Table 2 constant. Figure 2a shows the NETs profile and the contribution of each NET on the removal rate. Only the options EW and Biochar are initially selected within the negative emissions target range of 2.18 to 4.80 Gt C eq./y. To further satisfy the increasing negative emissions target above 4.80 Gt C eq./y, the model eventually taps DAC and BECCS. EW is given the highest overall priority on the negative emissions allocation among the NETs. EW has the highest land use intensity (1.22 ha/t C eq.) and energy input (3 GJ/t C eq.) but has insignificant nutrient requirements compared to the other NETs. The observed prioritization is probably due to the more binding nutrient constraints and the more relaxed land use and energy input constraints. To illustrate, the land use, water use, and energy input in Figures 2b, 2c, and 2d begin below their respective maximum values and increase with the increasing negative emissions target until the resource limits are reached. On the other hand, Figures 2e and 2f show that both nitrogen and phosphorous requirements are already at their maximum values in the entire range of the negative emissions target, although the value decreases for phosphorous from targets of 5.67 Gt C eq./y and above.

EW takes the biggest allocation for land use and energy input in Figures 2b and 2d. Because EW has a relatively low water use intensity (1.5 m³/t C eq.) it takes an insignificant allocation for water in Figure 2c compared to DAC and BECCS. Biochar and BECCS generate energy instead of consuming it, occupying the negative region in Figure 2d. Both EW and DAC have desirably zero impact on the nitrogen and phosphorous requirements, but EW has a lower cost (USD 92/t C eq.) compared to DAC (USD 1,600/t C eq.) which is the reason why EW was selected over DAC despite both having insignificant nutrient requirements and high energy input.

In terms of cost, the value increases slowly within the range of 2.18 to 4.80 Gt C eq./y and increases rapidly above this value (Figure 2g). DAC, which has the highest cost among NETs (USD 1,600/t C eq.), is included at a negative emissions target of 4.80 Gt C eq./y and above, explaining the rapid increase in the cost above this target. On the other hand, Biochar contributes to negative costs or cost savings and occupies the negative region in Figure 2g.

5.2 Effect of varying resource constraints

Each resource constraint was varied in its effective range while keeping all the other resource constraints constant using the values in Table 2 and targeting negative emissions at 6.54 Gt C eq./y. Figure 2h shows the effect of varying resource constraints on the total cost. The regions on the left of each curve are infeasible regions in the model. In general, tightening the resource constraints increases the total cost, and relaxing each resource constraint decreases the total cost until a constant value is reached, except for the water use constraint which stays constant at USD 3,196 x 10^9 /y. The effective ranges found for the rest of the resource constraints are, for land use, 24 to 593 Mha; energy input, 3.9 to 12.7 EJ/y; nitrogen requirement, 1.87 to 4.72 Mt/y; and phosphorous requirement, 0.14 to 0.81 Mt/y. The lower limits in each effective range give the lowest possible value for that resource constraint, below which yields an infeasible solution in the model. On the other hand, the higher limit in the effective range gives the highest value above which the total cost remains constant. The total cost ranges from USD 552 x 10^9 to 10,151 x 10^9 /y as shown in Figure 2h.



Figure 2: Effect of varying negative emissions target on the (a) NET profile, (b) land use, (c) water use, (d) energy input, (e) nitrogen requirement, (f) phosphorous requirement, (g) total cost; and (h) the effect of varying resource constraints on total cost

6. Conclusions

A superstructure model has been developed for optimizing NETs under resource constraints. The model gives the optimal portfolio of NETs and their recommended capacities while minimizing the cost and achieving a negative emissions target. The model also ensures that the selected NETs perform under the given resource limits. A scenario where six terrestrial NETs (BECCS, AR, SCS, Biochar, DAC, and EW), and five resource constraints (land, water, energy, nitrogen, and phosphorous requirements) was investigated targeting negative emissions of 6.54 Gt C eq/y. The model is able to identify a NETs portfolio consisting of BECCS, Biochar, DAC, and EW while meeting the resource constraints for a total cost of USD 3,195.67 x 10⁹/y. Varying the negative emissions target results to different NET portfolios, and for each portfolio, EW is given the highest priority due to the more binding nutrient constraints and the more relaxed land use and energy input constraints. Although EW and DAC have similar resource impacts, EW is selected over DAC because of its lower cost (92 USD/t C eq) compared to DAC (1,600 USD/t C eq). In general, tightening the resource constraints increases the total cost, and relaxing each resource constraint decreases the total cost until a constant value is reached. A superstructure model can provide support in decision-making when selecting a portfolio of NETs for large-scale implementation under resource constraints. The model has the following limitations which may be considered in future work, incorporating the uncertainties in the impacts of NETs on the resources, uncertainties in the resource limits, additivity/mutual exclusivity of NETs, and permanence of NETs in the model are recommended.

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