

Bilevel Programming for Optimizing Carbon Dioxide Removal Portfolios

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Purchase of carbon dioxide removal (CDR) credits is an important decarbonation option for many firms seeking to reach net zero emissions. These credits can supplement other decarbonization measures by offsetting hard-to-abate emissions. However, carbon markets are currently dominated by low-quality CDR credits generated by techniques with low durability or sequestration permanence. Companies tend to favor these credits due to their low cost compared to more durable CDR produced using novel technologies such as direct air capture (DAC). As a result, CDR portfolios tend to consist of credits with dubious climate change mitigation value. In this work, we develop a bi-level mathematical program to model how government can use economic incentives to induce industry to select portfolios that favor durable CDR. The model is demonstrated using an illustrative case study. In the Stackelberg solution, the government's objective is only 6.9 % lower than the maximum benefit, while the cost for the industry is 43 % lower than if the government decision was fully in control. The model calibrated the optimal total CDR ratio, durable CDR ratio, and emissions violation ratio, which demonstrates the model's importance in developing policy instruments.

1. Introduction

A mix of decarbonization techniques will be needed to achieve global net zero ambitions and keep climate change within safe limits (IPCC, 2022). The main decarbonization measures being considered in scientific and policy discourse are replacement of fossil fuels with renewables, enhancement of energy efficiency, carbon capture, utilization, and storage (CCUS), and carbon dioxide removal (CDR) (Glavina et al., 2025). The latter entails the deliberate sequestration of carbon from the atmosphere using a variety of negative emissions technologies (NETs), which range from nature-based to engineered approaches (Minx et al., 2018). For example, afforestation, soil carbon sequestration, and blue carbon management rely on photosynthesis to fix carbon in live or dead biomass. Biochar sequestration uses intermediate thermochemical processing to stabilize the biomass and improve sequestration permanence or "durability." Alternatively, the biomass can be burned in bioenergy with CCUS (BECCUS) systems. Enhanced weathering relies on accelerated geochemical reactions to store carbon as bicarbonate ions in water. Direct air capture uses separation processes to skim CO₂ from the atmosphere and subsequently store it in geological reservoirs. CDR techniques have their individual advantages and drawbacks (Mac Dowell et al., 2022). It is anticipated that CDR will eventually become a major part of the world's decarbonization efforts (Mannion et al., 2023) which can influence the uptake of both firms and countries (Green et al., 2024). However, current levels of deployment remain low and dominated by non-durable techniques (Lamb et al., 2024) suggesting that commercialization pathways for CDR should be supported by adequate policies throughout the entire project development (Hickey et al., 2023).

Decision-support models will be needed for effective deployment of CDR technologies (Migo-Sumagang et al., 2023). A portfolio optimization approach can be used since multiple NETs may be needed to meet decarbonization targets within system-specific constraints; it will also be necessary to model the presence of multiple decision-making agents (Tan et al., 2022). In particular, models can be used to calibrate CDR policies to influence industry decisions (Edenhofer et al., 2024). Corporate decarbonization efforts currently make extensive use of low-durability CDR (Caldecott and Johnstone et al., 2024) with overrated climate change mitigation value (Brunner et al., 2024). Process integration techniques can be used to integrate CDR quality

when planning CDR deployment systems (Tan et al., 2025). Stackelberg or leader-follower games can be used to develop more effective government policies to induce greater use of durable CDR in industry. Such games can be formulated as bilevel mathematical programs (Bracken and McGill, 1973), in which the follower's optimization model is nested inside the leader's model. There is extensive literature on the applications and algorithmic aspects of such models (Sinha et al., 2018); however, the only published use of Stackelberg games on CDR deployment is the bilevel model by Tapia et al. (2023) for enhanced weathering supply chains. There are no reported works on bilevel optimization of CDR portfolios in the scientific literature.

To address this research gap, a novel bilevel linear programming (BLP) model is developed in this work for optimizing CDR portfolios. In the model, government seeks to maximize the public benefits of decarbonization by setting targets on total CDR and durable CDR to be implemented by industry; industry then seeks to find the CDR portfolio that minimizes cost, including penalties for the violation of the mandated CDR targets. This decision-making hierarchy is illustrated in Figure 1. Solving the model gives the government's Stackelberg strategy (i.e., the policy that gives the greatest public benefit given industry's cost-minimizing behaviour). The rest of the paper is organized as follows. Section 2 gives the formal problem statement. Section 3 discusses the model formulation and the solution procedure based on the grid search algorithm (Bard, 1983). Section 4 demonstrates the model on an illustrative case study. Section 5 gives the conclusions and promising future research directions.

2. Problem Statement

The formal problem statement is given as follows:

- Given a leader–follower game where the government acts as the leader and the industry as the follower;
- Given that the leader seeks to maximize the total monetized public benefit of decarbonization by setting separate targets for total CDR and durable CDR to be used by industry;
- Given that the follower seeks to minimize its total CDR cost plus penalty payments for violating the government-mandated targets;

It is further assumed that:

- The external cost and emissions penalty per unit of CO₂ are fixed, but not necessarily equal to each other;
- The government is willing to tolerate a small violation of its CDR targets, subject to penalty payments;
- Multiple CDR options are available, each with its own cost and permanence factor;
- The government classifies a subset of the CDR options as durable, and specifies a separate target for their use;
- Industry selects its portfolio based only on nominal CDR (i.e., without considering the permanence factor).

The goal is to determine the government's Stackelberg strategy, which is the set of policies that maximizes public benefit subject to industry's cost-minimizing response.

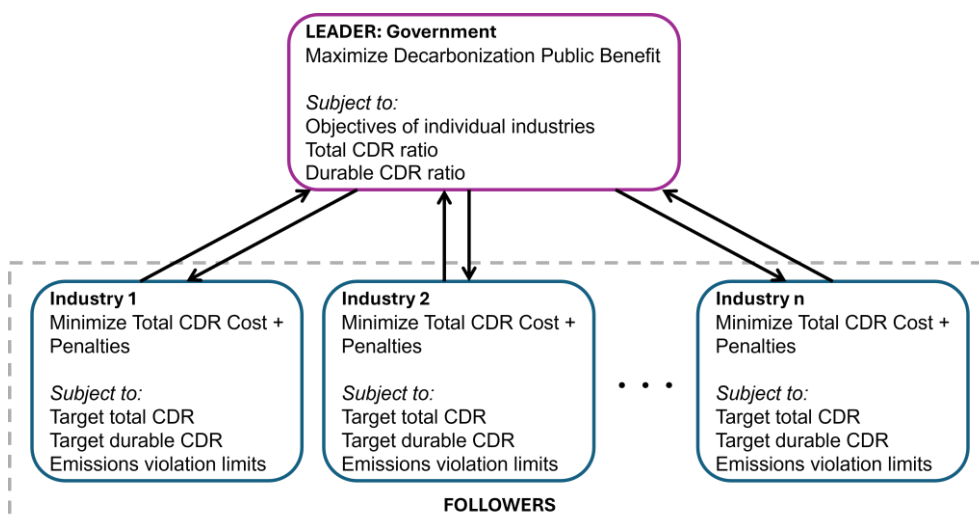


Figure 1: Decision-making hierarchy for the bilevel programming problem.

3. Model Formulation and Solution Algorithm

The objective of the leader is to maximize public benefit as given in Eq(1), where the first term corresponds to the benefit derived from the sequestered CO₂ while the second term is the value generated by the government resulting from penalties paid by the industry due to excess emissions. The model should select which CDR technologies should be implemented and at what levels (x_i). The government prefers technologies with higher climate repair or durability coefficient (A_i) which is an indicator of the permanence of CO₂ sequestration. A higher durability coefficient means that the captured carbon is reliably sequestered for longer periods of time. E is the social cost of carbon. P is the unit penalty cost for excess carbon, Z is the baseline emission of the company, and v is the fractional emission violation. The leader's objective is subject to the follower's objective function (Eq(2)) which is to minimize the costs incurred by the industry resulting from CDR and from penalties due to excess emissions. The total CDR implemented should meet the identified target CO₂ removal ratio, r , within allowable violation limits, v_r (Eq(3)). The amount of CDR from durable sources should also exceed the identified target removal ratio from durable CDR, q , (Eq(4)), where B_i is binary and indicates which of the CDR technologies are considered durable and v_q is a violation when the quality requirement of the government is not met. The overall violation penalty will be the higher value between v_q and v_r (Eq(5)). The variables q , r , v_q , v_r , and v should be within defined upper and lower limits as shown in Eq(6) to Eq(8). The implementation of each CDR technology i (Eq(9)) as well as the total amount of CDR implemented cannot exceed the baseline emissions (Eq(10)).

$$\max \left(\sum_i^n A_i x_i \right) E + PZv \quad (1)$$

s. t.

$$\min \sum_i^n C_i x_i + PZv \quad (2)$$

$$s. t. \quad \sum_i^n x_i = Z(r - v_r) \quad (3)$$

$$\sum_i^n B_i x_i = Z(q - v_q) \quad (4)$$

$$v = \max\{v_q, v_r\} \quad (5)$$

$$q^{LL} \leq q \leq q^{UL} \quad (6)$$

$$r^{LL} \leq r \leq r^{UL} \quad (7)$$

$$v^{LL} \leq v, v_r, v_q \leq v^{UL} \quad (8)$$

$$x_i \leq Z \quad \forall i \quad (9)$$

$$\sum_i^n x_i \leq Z \quad (10)$$

To solve Eq(1) to Eq(10), the grid search algorithm proposed by Bard (1983) is used. Here, a parameter λ is introduced to integrate the two objectives (Eq(1) and Eq(2)) resulting in the new objective function indicated in Eq(11). The solution is then obtained using the grid search algorithm developed by Bard (1983):

Step 1: Set $\lambda = 1$ and solve Eq(11) subject to constraints Eq(3) to Eq(10) to determine r^1 , q^1 , v^1 and x_i^1

Step 2: Check the feasibility of the inner problem (Eq(2) – Eq(10)) using r^1 and q^1 to determine \bar{v} and \bar{x}_i . If $\bar{x}_i = x_i^1$ and $\bar{v} = v^1$, stop. Otherwise move to Step 3.

Step 3: Determine the minimum value of λ such that r^j , q^j , v^j and x_i^j remains optimal and assign it as λ_{\min} . Identify the next value $\lambda_{j+1} = \lambda_{\min} - \delta$, with $\delta > 0$ and sufficiently small so that no vertices are missed.

Step 4: Solve Eq(11) subject to constraints Eq(3) to Eq(10) and determine r^{j+1} , q^{j+1} , v^{j+1} and x_i^{j+1} .

Step 5: Check the feasibility of the inner problem (Eq(2) – Eq(10)) using r^{j+1} and q^{j+1} to determine $\overline{v^{j+1}}$ and $\overline{x_i^{j+1}}$. If $\overline{x_i^{j+1}} = x_i^{j+1}$ and $\overline{v^{j+1}} = v^{j+1}$, stop. Otherwise move to Step 3.

$$\max(\lambda) \left[\left(\sum_i^n A_i x_i \right) E + PZv \right] - (1 - \lambda) \left[\sum_i^n C_i x_i + PZv \right] \quad (11)$$

The model is implemented in LINGO 20.0 (Schrage, 2003) using a laptop with 11th Gen Intel(R) Core(TM) i5-1135G7 @ 2.40GHz processor with 16.0 GB RAM. Model results were obtained in 0.20 seconds.

4. Case Study

The case study considers an industry with baseline emissions of 100 t CO₂ which seeks to reduce its emissions by buying CDR credits from four available technologies with cost and durability coefficients shown in Table 1. The total amount of credits that can be bought cannot exceed the baseline emissions. The reduction obtained from durable CDR, all CDR technologies selected, and violation due to excess emissions as a proportion of the baseline emissions should be kept within defined lower and upper limits indicated in Table 2. In practice, the durability factors can be based on concepts such as climate repair value (Prado and Mac Dowell, 2023) or time-weighted sequestration (Wenger et al., 2022). The social cost of carbon is 200 US\$/t while the penalty cost for excess emissions is 150 US\$/t. If there were no policies or constraints to the industry, they will continue emitting at their baseline emissions level. The government can influence the behavior of the industry by putting in place policies. The government (leader) can choose the required level of total emissions reduction (r), and the proportion obtained from durable CDR (q). The follower can then decide which CDR technology credits to purchase to minimize their total cost while considering the constraints set by the leader.

Table 1: Cost and durability coefficients of CDR technologies

CDR Technology	Cost (in US\$/t), C_i	Durability coefficient, A_i
Afforestation/Reforestation (AR)	60	0.15
Biochar (BC)	120	0.40
Enhanced Weathering (EW)*	200	0.92
Direct Air Capture (DAC)*	350	0.95

*durable CDR

Table 2: Lower and upper limits of reduction ratio, quality CDR, and violation

Variable	Lower Limit	Upper Limit
q	0.2	1.0
r	0.8	1.0
v	0.0	0.1

To obtain the objective of the leader, Eq(11) is solved subject to constraints in Eq(3) to Eq(10) with $\lambda = 1.0$. This results in the government setting $q = 1.0$ and $r = 1.0$ which indicates full emissions reduction and possibly sourcing all credits from durable CDR. However, the government would prefer that the company obtain just 90 tCO₂ CDR credits from DAC and 10 tCO₂ credits from BC to maximize its overall benefit. Similarly, the objective of the follower is determined by solving Eq(11) subject to Eq(3) to Eq(10) with $\lambda = 0.0$. Here, the solution results in $q = 0.2$, $r = 0.8$, and $v = 0.1$ which is desirable to the industry since the required reduction targets are at the lowest possible level. This enables the industry to purchase 60 tCO₂ credits from the cheapest source AR, and 10 tCO₂ credits from the cheaper durable CDR EW. This is far from the intended result of the leader or government. The Stackelberg solution is then determined using the procedure outlined in Section 3 and was obtained when the value of $\lambda = 0.59$. The resulting optimal solutions are summarized in Table 3.

Results indicate that the Stackelberg solution is for the government (leader) to set the target emissions reduction $r = 1.0$ with $q = 1.0$ indicating that total reduction should be implemented and that all should be sourced from durable CDR. The rational reaction of the industry (follower) is to buy 90 tCO₂ of CDR credits generated from EW leaving 10 tCO₂ as excess emissions ($v = 0.1$). The government obtains an objective function of US\$ 18,060 which is only 6.9 % lower than the maximum benefit if the government was entirely under control. The industry on the other hand needs to spend US\$ 19,500 to reduce its emissions and meet the standards set by the government. This solution is higher than the lowest cost of US\$ 7,100 that can be obtained if the industry had full control of the situation. However, the Stackelberg solution is 43 % lower in cost than if the government

decision was implemented. The industry was able to select the durable CDR credit with lower cost. This solution meets the objective of the government to adopt durable CDR while moderating the cost to the company.

Table 3: Comparative solutions for leader, follower, and the Stackelberg Solution

Variable	Leader	Follower	Stackelberg Solution
q	1.0	0.2	1.0
r	1.0	0.8	1.0
v	0.1	0.1	0.1
x(AR)	0	60	0
x(BC)	10	0	0
x(EW)	0	10	90
x(DAC)	90	0	0
Leader's objective	19,400	5,140	18,060
Follower's objective	34,200	7,100	19,500

5. Conclusions

A novel BLP model was developed in this work for optimizing the deployment of CDR techniques in industry. The model captures government-industry interactions in a Stackelberg game involving the use of CDR credits for industrial decarbonization. The government seeks to maximize the benefit to the public by adjusting mandated targets for total and durable CDR, subject to industry's optimal response; industry chooses the CDR portfolio that minimizes its total cost, including penalties for violating mandated limits. The model is demonstrated with an illustrative case study. The results suggest ways to rigorously calibrate policy instruments to maximize climate change mitigation benefits of CDR use in industrial decarbonization.

Future work can extend the model by incorporating a broader range of decarbonization techniques and policy instruments that may entail introducing nonlinearities and integer variables. The impact of variations in penalty cost and baseline emissions resulting from different industry types can also be explored. New algorithms will then be needed to solve these more complex models.

Nomenclature

Leader's decision variables

q – Durable CDR ratio

r – Total CDR ratio

Follower's decision variables

v – Emissions violation ratio

v_q – Violation due to CDR durability

v_r – Violation due to total CDR requirements

x_i – CDR credit from technology i

Parameters

λ – 0 to 1

A_i – durability coefficient of CDR technology i

B_i – indicator of high-quality CDR

C_i – cost of CDR credit from technology i, US\$/t

E – social cost of carbon, US\$/t

P – penalty cost, US\$/t

q^{LL} , q^{UL} – lower and upper limits of high-quality CDR

r^{LL} , r^{UL} – lower and upper limits of emissions reduction

v^{LL} , v^{UL} – lower and upper limits of emissions violation

Z – baseline emissions, tCO₂

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