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Bilevel Optimization of Enhanced Weathering Networks with P-graph

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Carbon dioxide removal (CDR) will be needed to offset residual greenhouse gas (GHG) emissions and achieve carbon neutrality. Enhanced weathering (EW) is a promising CDR technique based on the acceleration of naturally occurring reactions between alkaline minerals with carbonic acid in rainwater. The reactive minerals are pulverized and then applied at a calibrated rate to terrestrial sites; the weathering reaction results in carbon sequestration as bicarbonate ions in the runoff water. EW can be deployed via carbon management networks (CMNs) of sources (mineral-crushing plants) and sinks (application sites). However, current CMN optimization models fail to account for the presence of multiple players (i.e., government and industry) with conflicting objectives. Bilevel optimization models can be used to account for these conflicts via leader-follower games. In this work, a P-graph approach to the optimization of EW-based CMNs is developed. The government is assumed to act as the leader seeking to minimize external costs to the public by specifying acceptable transport routes for mineral powder; the industry is assumed to act as the follower seeking to maximize its CDR earnings by minimizing its costs subject to the transport network topology constraints. Note that the government imposes the latter constraints in anticipation of the industry's intent to maximize revenues. The model is implemented as a Python code and demonstrated with an illustrative case study. Results show that by following the Stackelberg solution, cost of transportation may be reduced by at least 5 % and the risk of death by 79 %.

1. Introduction

The current climate crisis can only be addressed with a mix of strategies that includes increasing the use of renewable energy, enhancing energy efficiency, and deploying Negative Emissions Technologies (NETs) (IPCC, 2022). NETs achieve Carbon Dioxide Removal (CDR) through different chemical, physical or biological mechanisms; carbon is sequestered either as CO_2 in geological reservoirs or in other forms in compartments such as biomass or minerals. Examples of NETs include direct air capture, bioenergy with CO_2 capture and storage, and less mature alternatives like Enhanced Weathering (EW) (Minx et al., 2018). In addition to CDR, the secondary environmental effects of large-scale use of NETs can be adverse or favourable (Smith et al., 2019). Optimized NET portfolios will be needed to balance global CDR benefits with local or regional sustainability issues (Strefler et al., 2021).

EW was first proposed as an engineered acceleration of natural weathering reactions between carbonic acid and silicates to sequester CO_2 (Seifritz, 1990). In ex situ EW, alkaline rocks or minerals are mined, reduced to a fine powder (~10 μm), sent to application sites, and allowed to spontaneously react with CO_2 dissolved in rainwater. Carbon is sequestered in the form of dissolved bicarbonate ions that are ultimately carried by runoff water into the sea. The CDR rate and efficacy are complex functions of particle composition and surface area as well as ambient conditions (e.g., precipitation, temperature, and soil chemistry) at the application site (Strefler et al., 2018). EW is a promising NET, but the CDR benefits need to be balanced with potential environmental impacts that can occur during the mining, grinding, transport, and application phases of the life cycle of both terrestrial (Eufrasio et al., 2021) and coastal EW (Foteinis et al., 2023). Surveys indicate that concerns about

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such impacts can be a significant barrier to the public acceptance of EW as a climate change mitigation technique (Spence et al., 2021).

Rigorous models and techniques, such as those based on Process Integration (PI), can also be used to facilitate decarbonisation planning (Klemeš, 2023). Mathematical Programming (MP) models have been proposed for optimising EW networks that are similar to supply chain or resource conservation networks (Tan and Aviso, 2019); however, the latter model and its current extensions do not consider the presence of multiple decision-making agents or players. Future EW networks will involve interactions between government regulators seeking to mitigate the localised risks (e.g., from vehicular accidents) or environmental impacts (e.g., from air pollutants) arising from hauling large quantities of material (Fan et al., 2018) and firms seeking to maximise revenues from CDR. The government needs to determine its Stackelberg solution, which is its best possible strategy in anticipation of the industry's self-interested actions. Such interactions result in leader-follower or Stackelberg games, which can be represented by bilevel MPs (Kalashnikov et al., 2015) where the follower's optimisation problem is nested within the leader's (Bracken and McGill, 1973). Solving such models is computationally challenging and has led to the development of various deterministic and heuristic algorithms for finding the Stackelberg strategy (Sinha et al., 2018). Bilevel MP models have been developed for planning transportation networks of hazardous materials, along with deterministic (Bianco et al., 2009) or heuristic (Erkut et al., 2008) solution algorithms. Newer variants of these models account for factors such as the risk appetite of decision-makers (Su and Kwon, 2020) and the choice of transportation mode (Fontaine et al., 2020). Despite these developments, the Stackelberg game approach has not yet been applied to EW networks, where CDR benefits need to be tempered with consideration of localised risks and environmental impacts.

This work addresses the research gap by developing a game-theoretic extension of the LP model for optimising EW networks (Tan and Aviso, 2019), considering government-industry interactions, as well as a P-graph-based algorithm for solving the resulting model. The latter is based on the procedure previously developed for a technology selection problem involving government and industry players (Tan et al., 2021). This work allows to identify potential routes with minimal costs and provides insights into transportation risks associated with it. The rest of this paper is organised as follows. Section 2 formalises the problem statement. Section 3 gives the model formulation, and Section 4 describes the P-graph-based solution algorithm. Then, Section 5 shows an illustrative case study on EW network optimisation. Finally, Section 6 gives the conclusions and recommendations for further research.

2. Formal problem statement

This work combines EW source-sink matching problem proposed by Tan and Aviso (2019) with the Stackelberg game model from Tan et al. (2021). The problem may be stated as follows:

- Given a set of sources (rock/mineral crushing plants);
- Given a set of sinks (EW sites);
- Given a transportation network consisting of links (road segments) and intermediate nodes (junctions) that connects the sources to the sinks;
- Given two rational players, i.e., the leader (government) and the follower (industry);
- Given that the leader seeks to minimise total risk from transporting crushed rock/mineral and controls access to links in the transportation network;
- Given that the follower seeks to maximise profit from CDR credits and selects a transportation plan (i.e., a set of routes) using the accessible links;

Linearity assumptions of conventional PNS problems are also assumed to hold. This assumption means that the transportation risk associated is proportional to the amount of resources being transported. The leader's problem is to determine its Stackelberg strategy – the set of accessible links in the transportation network that minimises total risk, subject to the follower selecting a profit-maximising transportation plan within the accessible part of the network.

3. Bilevel model formulation

The leader's objective is to minimise the total risk associated with the transport of crushed minerals to the EW sites as indicated in Eq(1), where r_j is the risk associated with using link j and x_j is the amount of material going through link j. The associated risk can relate to events such as the potential for damage from accidents and the exposure of communities to EW particulate emissions. Eq(2) indicates that the activation of link j, β_j, is a binary variable. The follower's objective is to maximise profit (Eq(3)). It is subject to transport connectivity constraints (Eq(4)), road network capacity limits (Eq(5)), and node output requirements (Eq(6)). Eq(7) ensures that the follower selects a link from the leader's preferred links. The follower's selection is represented by the binary variable, b_j (Eq(8)). In the special case where the follower's binary variable takes the same value as the leader's binary variable, the lower-level problem can be reduced to an LP model as in Tan et al. (2021).

Leader's objective $$\min \sum_{i=1}^{m} r_i^P y_i + \sum_{j=1}^{n} r_j^V x_j \quad (1)$$

Subject to:

$$\beta_j \in \{0,1\}^n \quad \forall j \quad (2)$$

Follower's objective: $$\min \sum_{i=1}^{m} c_i^P y_i + \sum_{j=1}^{n} c_j^V x_j \quad (3)$$

subject to:

$$y_i = \sum_{j=1}^{N} a_{ij} x_j \quad \forall i \quad (4)$$

$$x_j \le b_j M \quad \forall j \quad (5)$$

$$y_i^L \le y_i \le y_i^U \quad \forall i \quad (6)$$

$$b_j \le \beta_j \quad \forall j \quad (7)$$

$$b_j \in \{0,1\}^n \quad \forall j \quad (8)$$

4. P-graph solution algorithm

P-graph is a graph theoretic framework for solving Process Network Synthesis (PNS) problems (Friedler et al., 2022). P-graph uses a bipartite graph representation with O-type nodes to denote processes and M-type nodes to denote materials or forms of energy; arcs signify how O-type and M-type nodes are linked to each other based on chemical or physical relationships. Five axioms are the basis for the rigorous development of algorithms in the P-graph framework (Friedler et al., 1992a). The Maximal Structure Algorithm (MSG) is used to assemble a complete and non-redundant maximal structure from individually specified process units (Friedler et al., 1993). The Solution Structure Algorithm (SSG) is used to enumerate combinatorially feasible network topologies for a given PNS problem (Friedler et al., 1992b). Both MSG and SSG rely only on structural information. Given additional flow data and techno-economic parameters, the Accelerated Branch-and-Bound (ABB) algorithm is used to determine the cost-optimal solution (Friedler et al., 1996). Alternative optimal and near-optimal solutions can also be readily generated for evaluation by the designer. In addition to the classical PNS problem in plant design, P-graph has also been used to solve a diverse range of mathematically analogous PNS-like problems (Friedler et al., 2019). A P-graph approach to solving a special class of bilevel optimisation problems was proposed by Tan et al. (2021).

In this work, the problem elements are mapped as follows. Junctions in a transportation network are represented as M-type nodes, while links between junctions are represented as O-type nodes. The sources and sinks are special types of M-type nodes corresponding to raw materials and products. Mass is conserved within any given link, but mixing or redistribution can occur at junctions. The capacity of a link can also have an upper bound. The specific risk per unit mass of material transported is defined for each link in the network, which reflects properties such as the distance between the start and end junctions, the proximity to the exposed population, or the historical accident frequency.

The P-graph-based solution procedure for solving this game is as follows (Tan et al., 2021):

- Use SSG to generate all combinatorically feasible transportation networks.
- Use the topology of each enumerated network to define constraints for the follower's MILP or LP for each local subproblem.
- Use the appropriate optimization algorithm (e.g., branch-and-bound or simplex) to solve each of the follower's local subproblems.

- Compute the leader's objective function or payoff at each of the follower's optimal solutions.
- Select the network (corresponding to the Stackelberg strategy) that gives the best payoff for the leader, subject to the optimisation of the follower's subproblem.

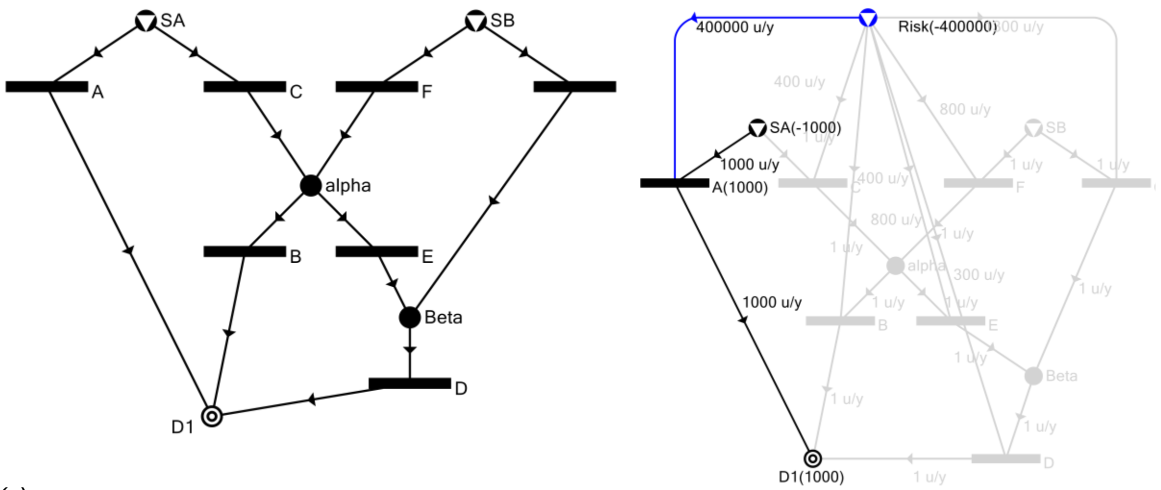
The fundamental procedure can also include the exploration of alternative optimal and near-optimal solutions for the follower's local subproblem and the leader's master problem. Alternative Stackelberg strategies that arise may be evaluated based on criteria not inherent in the main algorithm. A case study is used to demonstrate this algorithm in the next section.

5. Illustrative case study

This case study has two rock-crushing plants and one application site connected by an intermediate transportation network with seven links and two junctions. The application site has a capacity of 1,000 t/d of rock, while source A (SA) has a maximum available crushed mineral of 1,000 t/d, and source B (SB) has a maximum available crushed mineral of 3,000 t/d. Illustrations are generated using P-graph Studio, but the computations are executed using original Python code (Tapia, 2023). Table 1 lists the leader's and follower's parameters for these links. In this case study, the leader seeks to minimise the risk of incremental deaths from road accidents. The follower seeks to minimise transportation costs, which are linked to the cost of fuel needed to traverse a given path. The maximal structure of the transportation network is shown in Figure 1. Each network generated by SSG defines a local subproblem for the follower, which in this case, is formulated as an LP model. The resulting optimal responses of the follower to these alternatives are listed in Table 2, along with the leader's payoff. The leader's Stackelberg strategy can be readily identified by direct inspection of the last column.

Table 1: Associated costs and risks to links and sources

Link	Cost per unit (€/t)	Risk per unit (10^{-6} deaths/t)	Source	Cost per unit (€/t)	Risk per unit (10^{-6} deaths/t)
A	10	200	SA	3	200
B	3	400	SB	2	300
C	4	200			
D	2	300			
E	2	800			
F	3	500			
G	5	1000			



(a)

(b)

Figure 1: Network structures for the EW network case study: (a) maximal structure and (b) the Stackelberg solution

Table 2: Alternative network structures and their performance

Network	A	B	C	D	E	F	G	Cost (€)	Risk (10^{-6} deaths)
1		1,000				1,000		27,400	1.20
2				1,000			1,000	27,300	1.60
3				1,000	1,000	1,000		27,300	1.90
4		1,000	1,000					26,300	0.80
5			1,000	1,000	1,000			26,200	1.50
6	1,000							26,000	0.40

Based on the alternative network structures, the Stackelberg solution is Network 6, where the incremental risk is 0.40×10^{-6} deaths, and the cost of transport is € 26,000. The results suggest that the minimum risks can be attained at the shortest possible route. However, Network 5 has a slightly lower risk than Network 2, even if Network 5 takes 3 routes. It is also preferred to transport resources from one resource point only. The reduction of alternative network structures from 39 networks to 6 networks shows the possible strategies that the follower may adopt, which the leader is anticipating. These results contribute to decision-making for minimising transportation costs and risk simultaneously.

6. Conclusions

A P-graph methodology has been developed for the game-theoretic optimisation of EW networks. This bilevel optimisation problem represents government-industry interactions as a leader-follower game, where the government makes discrete decisions on available routes while the industry optimises its EW operations within the resulting transportation network. The government seeks to minimise local risks (e.g., from air pollutants or potential accidents) from the hauling of EW materials, while the industry seeks to maximise revenues generated from CDR credits. The interaction results in a bilevel MILP model whose Stackelberg strategy can then be found using the modified P-graph methodology. A demonstration case study implemented in Python is solved to illustrate this new approach; note that the Stackelberg strategy is not necessarily Pareto-optimal.
Future work can explore either computational enhancements or new applications. Computational enhancements can include non-linear payoff functions and case-specific topological constraints for either player. New applications can focus on emerging environmental concerns, such as reverse supply chains for recycling plastic waste within a CE framework.

Nomenclature

Parameters:
a_{ij} – connectivity of node i with link j
c_i^P – cost associated with CO_2 emissions from source i
c_j^V – variable transport cost associated with link j
r_i^P – associated risk to source i
r_j^V – associated risk to link j
x_j^U – maximum flow in link j
y_i^L – lower limit to the output of node i
y_i^U – upper limit to the output of node i

Variables:
β_j – leader's binary variable in selecting link j
b_j – follower's binary variable in selecting link j
x_j – follower's flow in link j
y_i – follower's net output for node i

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