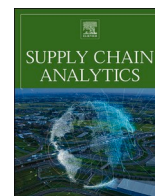


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A quadratic-linear bilevel programming approach to green supply chain management

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ABSTRACT

Green Supply Chain Management requires coordinated decisions between the strategic and operational organization layers to address strict green goals. Furthermore, linking CO₂ emissions to supply chain operations is not always easy. This study proposes a new mathematical model to minimize CO₂ emissions in a three-layered supply chain. The model foresees using a financial budget to mitigate emissions contributions and optimize supply chain operations planning. The three-stage supply chain analyzed has inbound logistics and handling operations at the intermediate level. We assume that these operations contribute to emissions quadratically. The resulting bilevel programming problem is solved by transforming it into a nonlinear mixed-integer program by applying the Karush-Kuhn-Tucker conditions. We show, on different sets of synthetic data and on a case study, how our proposal produces solutions with a different flow of goods than a modified linear model version. This results in lower CO₂ emissions and more efficient budget expenditure.

1. Introduction

Climate change is the toughest challenge for humanity, requiring a paradigm shift in the planning and operation of almost all human activities. Minimizing CO₂ emissions has been progressively taken as an objective for the design and planning of operations, but it is now clear that even a simple minimization is not sufficient. The new paradigm is to pursue near-zero emissions in a medium-time horizon. This target is called carbon neutrality and is due by 2050 by several institutions such as the European Commission, which set an ambitious intermediate target of reducing emissions of 55% by 2030 compared to 1990 levels European Commission [15,16]. In these settings, Green Supply Chain Management requires a rethinking in organizational and collaboration settings with particular emphasis on Green Supply Chain Network Design (GrSCND). Green supply chain management emerged when companies were encouraged to implement innovative environmental management practices [42]. As analyzed by Khanal et al. [24] there is a strong mediating role between business performance and GSCM practices considering the multidimensional organizational impacts of practice implementation, employee job satisfaction, operational efficiency, relational efficiency, and organization performance. Recently, several works recorded how GSCM practices are becoming a must in industry

and societies. Özşkın and Görener [34] use multicriteria decision-making approach to individuate barriers for GRSCM. Jum'a et al. [23] put in relation GSCM with total quality management, while Pham et al. [36] use maturity models to analyze relations between digitization and GSCM.

Even though GrSCND is a research topic that is being increasingly studied in the literature, as demonstrated, for example, by the review of Waltho et al. [39] new models that consider structural elements and multiple objective functions. Most of the work on GrSCND addresses emissions control in the design of supply chain networks with specific attention to the transport phase only; a few papers address other emissions sources such as manufacturing, handling, and processing of raw materials. Moreover, accounting is done most of the time using linear functions; nonlinear aspects are rarely addressed. Nonlinear cost functions are considered, in particular, in transport, considering the impact of factors such as weight and velocity on emissions.

In Liotta et al. [28], the emissions are considered linearly in both production nodes and multimodal transport links. Additionally, Liotta et al. [27] analyze the problem of coordination between transport operators and the impact on emissions. The resulting problem is solved through an optimization-simulation approach. Porkar et al. [37] propose a mathematical programming model to maximize profit in a green

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supply chain with forward and reverse flows. In Coskun et al. [10], the attention is posed on the consumers which are segmented by a green expectations level, and the resulting network design problem is modeled as a mixed-integer programming model solved by a commercial solver. Multi-objective GrSCND considers Pareto efficient calculation of network designs in terms of costs and emissions as in Bouzembrak et al. [4] and in Wang et al. [40]. In Miranda-Ackerman et al. [32], emissions are calculated employing life cycle analysis, and network design is applied to a food processing company. The resulting multi-objective optimization model is solved by the application of a non-dominated sorting genetic algorithm.

Nonlinear functions are considered in Bektaş and Laporte [3], and piecewise functions in Fahimnia et al. [17] where a tactical problem is analyzed, and the authors evaluate the economic and environmental trade-offs in manufacturing and distribution planning. Concerning network nodes, emissions have been defined proportionately to production/warehousing capacity, as in Abdallah et al. [1]. In Saif and Elhedhli [38] the authors use a concave function to model warehouse emissions (linked to warehouse volume). The network design problem is then solved using a Lagrangian approach. A similar approach is used in Elhedhli and Merrick [14], where the relation between emissions and vehicle weight is assumed to be concave. In a recent work Caramia and Stecca [8], emissions are considered non-linearly in a two-layer supply chain design problem considered as a one-stage decision problem.

The modeling of emissions considering nonlinearities is more appropriate in several applications. In particular, is demonstrated by several studies how emissions are inversely related to green investments. The study of Li et al. [26] analyzed Chinese industries measuring the short and long-term green investments elasticity of carbon emissions and showed that increasing by 1% the level of the green investments conducts to a 0.071% and a 0.085% reduction of the short and long-term carbon emission levels, respectively. Analogous conclusions have been drawn by Luo et al. [29]. Nonlinearities appear when the accumulation effect of production and material management in a facility is considered. Several papers, such as Caramia and Stecca [8], and Wang et al. [40] use realistic case studies to study supply chains where technology and quantity processed affect emissions. The specific emissions quantity depends on the industry. For example in manufacturing, the study of Wang et al. quantifies the emission of milling machines in the manufacturing industry. In the work of Caramia and Stecca [9] consider multiperiod budget allocation problem when investment must be assigned to scheduling green projects over time.

When considering strategic decisions in green supply chains it is important to evaluate how to allocate investments and how to split them between efficiency increasing and emission decreasing. In our work we assess exactly this topic. In this regard, there is an emergent discipline called green finance studying these topics. Several papers address the budgeting problems in empirical ways. In the study of Huang [22], a Data Envelopment Analysis study is used to analyze and quantify the effects of green investments on industrial performance in an Asian country. Other authors, such as Luo et al. [30], and Caramia and Dell'Olmo [7] use mathematical models to compute optimal green investment decisions in green supply chains.

In this work, we present a novel GrSCND model to investigate the non-linear effects of operations on carbon emissions, in particular in network nodes. The model foresees using a financial budget to mitigate emissions and optimize the planning of supply chain operations. The three-echelon supply chain analyzed has inbound logistics and handling operations at intermediate levels. The resulting model is a Bilevel Programming Problem (BPP) in which the leader attempts to maximize his/her objective function by selecting a strategy that anticipates the reactions of the followers. The BPP so defined is solved by its transformation into a nonlinear mixed-integer programming model by applying the Karush-Kuhn-Tucker (KKT) conditions. Moreover, since in our model operations contribute to emissions quadratically, to show its effectiveness, we compare its performance to that of the same model that

implements a linear computation of the emissions. Furthermore, stability issues that typically arise in bilevel programming are addressed. The computational results, carried out using a commercial solver, reveal the effectiveness of the approach for strategic planning and decision-making related to budget allocation in supply chain efficiency and sustainability.

BPP [11,12] has been used to represent a wide variety of problems in which a leader sets decision variables that affect the decision domain and the optimal solution of a follower. BPP is strongly NP-hard even in the linear case [20]. The hierarchical structure of the problem can be converted into a standard mathematical program through the KKT conditions on the follower problem. The resulting problem is still non-convex even for linear and quadratic problems. Several solving procedures have been proposed, such as branch and bound, e.g., in [2,11,12,20,33]. Concerning GsSCND, in Caramia and Dell'Olmo [7] bilevel programming is used to minimize carbon emissions and transportation costs when both are modeled as linear functions. In Ghomi-Avili et al. [18], bilevel programming is used to represent competing supply chains where demand is uncertain and costs consider linear emission factors, while in Ghomi-Avili et al. [18] uncertainty is modeled using fuzzy sets. In Hassanpour et al. [21] and Golpi'ra et al. [19], robust optimization theory is used to represent uncertainty. In Hassanpour et al. [21], the leader is the organization that aims to maximize collection rates, while the follower maximizes the profit of the supply chain and decides the design of the closed-loop supply chain activating the reverse flow, which reduces carbon emissions. The problem is solved using a heuristic approach based on particle swarm and genetic algorithms. In Golpi'ra et al. [19], the authors use bilevel programming to model a vendor-managed inventory policy, robust optimization to take into account value at risk for the follower, and emissions are controlled linearly. Panja and Mondal [35] present a bilevel programming model for greening activities based and credit policies where inventory is crucial. Recent works on bilevel programming are applied to green supply chains and sustainability considering specific aspects such as customer selection [5], resource management [31], or product family [41].

The framework of the analyzed literature shows little or no attention to the nonlinear treatment of carbon emissions and no consideration of investments to neutralize the latter, especially in a bilevel programming setting. In our paper, we try to fill this literature gap in a twofold direction: (i) by analyzing the nonlinearity of CO₂ emissions of a facility defined as a function of the investment made in that facility and the flow entering the facility (reasons are properly detailed in Section 2) and (ii) by proposing a hierarchical formulation where the operational problem related to routing commodities from suppliers to customers, minimizing transportation and handling costs, is nested in an upper lower strategic problem associated with an investment to be made in green technologies to promote sustainability.

Moreover, the model proposed in this paper generalizes the formulation given in Caramia and Dell'Olmo [7] for a similar problem with the following improvements that generate a completely different model:

- in Caramia and Dell'Olmo [7], the authors proposed a linear-linear bilevel formulation, while in this paper we propose a quadratic-linear bilevel formulation;
- in this paper, we assume that the available budget for environmental protection depends on the cost of capacity installation of the facilities;
- in the proposed model, we added two additional constraints to strengthen the formulation.

The remainder of the paper is organized as follows. Section 2 details the formulation of the BPP. Section 3 discusses computational results and, finally, Section 4 reports conclusions and future work.

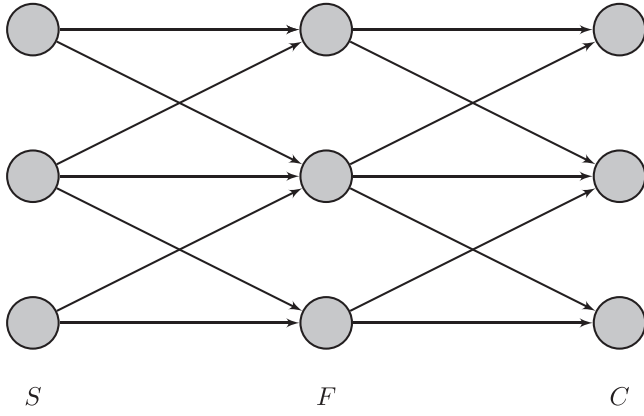


Fig. 1. A generic network representing a three-stage supply chain.

2. Problem definition and mathematical formulation

In this section, we describe the mathematical formulation of our problem. Given is a supply chain network modeled by a graph $G = (N, A)$, where N is the set of nodes and A is the set of arcs. Here, N encompasses three sets: the set S of suppliers, the set F of facilities, and the set C of customers, that is, $N = S \cup F \cup C$. The set A of arcs represents the connections among pairs of nodes belonging to the Cartesian products $S \times F$ and $F \times C$. Fig. 1 depicts the G graph. Given customer demands, supplier supply capacities, and a budget b_j for each facility to invest in environmental protection, the goal is to decide (i) which facility $j \in F$ must be opened along with the associated investment, (ii) which handling capacity must be installed in each opened facility, (iii) which supplier should be used, and (iv) how to distribute the products, taking into account CO₂ emissions in each process of the entire network.

The sets and parameters are as follows:

- P : the set of products (index p);
- S : the set of suppliers (index k);
- F : the set of facilities (index j);
- C : the set of customers (index c);
- N : the set of nodes of the supply chain network (index i);
- d_c^p : the demand of product $p \in P$ by customer $c \in C$;
- s_k^p : the supply capacity of supplier $k \in S$ for product $p \in P$;
- $ct_{i,i}^p$: transportation cost for product $p \in P$ from node $i \in N$ to node $i \in N$;
- r_j^p : capacity consumed by handling a unit of product $p \in P$ in facility $j \in F$;
- h_j^p : handling cost of product $p \in P$ in facility $j \in F$;
- $e_{i,i}^p$: amount of CO₂ emissions generated by each unit of flow associated with product $p \in P$ on arc $(i, i) \in A$;
- b_j : budget for investment of equipment for environmental protection in facility $j \in F$;
- ch_j : the unit handling capacity installation cost in facility $j \in F$.

The decision variables are as follows.

- $x_{i,i}^p$: the flow of product $p \in P$ from node $i \in N$ to node $i \in N$;
- z_j : the environment protection investment in facility $j \in F$;
- u_j : the handling capacity in facility $j \in F$.

When it comes to sustainability and CO₂ emission reduction, in the literature typically two objectives come into play: one is the overall cost of routing commodities over the supply network and the other is to minimize the overall CO₂ emissions and these two goals are used to build a bi-objective problem. This is not the case for our paper, where we

model the hierarchy between these two objectives. On the one hand, we have the operational problem related to routing commodities from suppliers to customers minimizing transportation and handling costs; on the other hand, we have a strategic problem associated with an investment to be made in green technologies to promote sustainability; this decision occurs before the system starts operating with transportation activities since technological transformation and installation require stopping production activities. Furthermore, we note that the decisions associated with the two objectives may not be, in general, pursued by either the same person or cooperative persons, since strategic decisions are under the facility governance, while transportation decisions may be managed by one or more than one company.

These reasons motivate the choice of adopting a bilevel model. Therefore, we have a leader (upper-level) decision-maker and a follower (lower-level) decision-maker. The leader is in charge of deciding on strategic aspects of the network, deciding about the handling capacity u_j to be installed in each facility $j \in F$ (in case the latter is zero then the facility is not opened) and the investment z_j to be made in each opened facility j to protect the environment, and aims to minimize the overall CO₂ emissions. The follower decision maker, instead, copes with the operational problem of determining optimal flows in the network (controlling variables $x_{i,i}^p$), after the leader has decided on variables u_j and z_j , $\forall j \in F$, to minimize the overall transportation cost.

The leader problem is as follows:

$$\min f_1 : \sum_{j \in F} \sum_{p \in P} w_j^p + \sum_{p \in P} \sum_{(i,i) \in A} e_{i,i}^p x_{i,i}^p \quad (1)$$

s.t.

$$x = \begin{cases} z_j + ch_j u_j \leq b_j, & \forall j \in F, \\ z_j \leq u_j M, & \forall j \in F, \\ u_j \geq 0, & \forall j \in F, \\ z_j \geq 0, & \forall j \in F. \end{cases} \quad (2)$$

The leader objective f_1 measures the total CO₂ emissions throughout the supply chain as follows. Variable z_j represents the investment made for environmental protection in facility $j \in F$. More specifically, higher values of z_j correspond to greater environmental investments in j and lead to lower CO₂ emissions at the same facility. On the other hand, given a value for z_j , the CO₂ emissions associated with j grow proportionally with the quantities of products handled in j . So, given $x_j^p = \sum_{k \in S} x_{kj}^p$, w_j^p is the function that measures CO₂ emissions based on both green investment level z_j and amount x_j^p of products p in j . In the next subsection, we will give the explicit definition of w_j^p . The leader constraint set x defines relations among investments and capacity. In particular, the first constraint in x is the budget constraint and limits the overall investment associated with the CO₂ emissions reduction equipment and the installed capacity in a facility j for every facility $j \in F$. The second constraint says that the investment z_j in j is zero if the latter facility is not opened (i.e., its capacity is zero); here M is a large number. The other two constraints define the domains of the variables.

The follower problem is:

$$\min f_2 : \sum_{p \in P} \sum_{(i,i) \in A} ct_{i,i}^p x_{i,i}^p + \sum_{p \in P} \sum_{j \in F} h_j^p \sum_{k \in S} x_{kj}^p \quad (3)$$

s.t.

$$Z = \begin{cases} \sum_{k \in S} x_{kj}^p - \sum_{c \in C} x_{jc}^p = 0, & \forall j \in F, \forall p \in P, \\ \sum_{j \in F} x_{jc}^p = d_c^p, & \forall c \in C, \forall p \in P, \\ \sum_{j \in F} x_{kj}^p \leq s_k^p, & \forall k \in S, \forall p \in P, \\ \sum_{p \in P} r_j^p \sum_{k \in S} x_{kj}^p \leq u_j, & \forall j \in F, \\ x_{i,i}^p \geq 0, \forall (i, i) \in A, & \forall p \in P. \end{cases} \quad (4)$$

The follower objective f_2 measures the total cost of the supply chain and consists of two parts, that is, the total cost of transportation and the

total cost of product handling. The follower constraint set Z defines relations among flow variables. In particular, the first constraint in Z is the flow conservation constraint. The second constraint states that the demands must be satisfied, while the third constraint ensures that, for each product $p \in P$, the amount of supply, from each supplier $k \in S$, should not exceed its supply capacity s_k^p . The fourth constraint requires that the processing requirement for handling all products in facility $j \in F$ does not exceed the capacity u_j of the facility. The remaining constraints define the domains of the variables.

The overall bilevel problem can be written as:

$$\begin{aligned}
 & \min \sum_{j \in F} \sum_{p \in P} w_j^p + \sum_{p \in P} \sum_{(i,i) \in A} e_{i,i}^p x_{i,i}^p \\
 & \text{s.t. } z_j + ch_j u_j \leq b_j, & \forall j \in F \\
 & u_j \geq 0, & \forall j \in F, \\
 & z_j \geq 0, & \forall j \in F, \\
 & x_{kj}^p, x_{i,i}^p \in \operatorname{argmin} \sum_{p \in P} \sum_{(i,i) \in A} ct_{i,i}^p x_{i,i}^p + \sum_{p \in P} \sum_{j \in F} h_j^p \sum_{k \in S} x_{kj}^p \\
 & \text{s.t. } \sum_{k \in S} x_{kj}^p - \sum_{c \in C} x_{jc}^p = 0, \forall j \in F, \forall p \in P, & (5) \\
 & \sum_{j \in F} x_{jc}^p = d_c^p, & \forall c \in C, \forall p \in P, \\
 & \sum_{j \in F} x_{kj}^p \leq s_k^p, & \forall k \in S, \forall p \in P, \\
 & \sum_{p \in P} r_j^p \sum_{k \in S} x_{kj}^p \leq u_j, & \forall j \in F, \\
 & x_{i,i}^p \geq 0, & \forall (i, i) \in A, \forall p \in P.
 \end{aligned}$$

2.1. The single-level reformulation

To solve this problem, we define the single-level problem obtained by replacing the follower problem with its optimality conditions. Indeed, the lower-level problem is a linear program and, therefore, its necessary and sufficient optimality conditions are given by primal feasibility PF , dual feasibility DF , and complementary slackness relations CS . To this end, we first define the dual variables associated with the follower constraints as follows:

- α_j^p : the dual variables associated with constraints $\sum_{k \in S} x_{kj}^p - \sum_{c \in C} x_{jc}^p = 0, \forall j \in F, \forall p \in P$;
- β_c^p : the dual variables associated with constraints $\sum_{j \in F} x_{jc}^p = d_c^p, \forall c \in C, \forall p \in P$;
- γ_k^p : the dual variables associated with constraints $\sum_{j \in F} x_{kj}^p \leq s_k^p, \forall k \in S, \forall p \in P$;
- δ_j : the dual variables associated with constraints $\sum_{p \in P} r_j^p \sum_{k \in S} x_{kj}^p \leq u_j, \forall j \in F$.

Primal feasibility PF :

$$\text{PF} = \begin{cases} \sum_{k \in S} x_{kj}^p - \sum_{c \in C} x_{jc}^p = 0, & \forall j \in F, \forall p \in P, \\ \sum_{j \in F} x_{jc}^p = d_c^p, & \forall c \in C, \forall p \in P, \\ \sum_{j \in F} x_{kj}^p \leq s_k^p, & \forall k \in S, \forall p \in P, \\ \sum_{p \in P} r_j^p \sum_{k \in S} x_{kj}^p \leq u_j, & \forall j \in F, \\ x_{i,i}^p \geq 0, & \forall (i, i) \in A, \forall p \in P. \end{cases} \quad (6)$$

Dual feasibility DF is:

$$\text{DF} = \begin{cases} \alpha_j^p + \gamma_k^p + r_j^p \delta_j \leq ct_{kj}^p + h_j^p, & \forall k \in S, \forall j \in F, \forall p \in P, \\ -\alpha_j^p + \beta_c^p \leq ct_{jc}^p, & \forall j \in F, \forall c \in C, \forall p \in P, \\ \alpha_j^p \in \mathbb{R}, & \forall j \in F, \forall p \in P, \\ \beta_c^p \in \mathbb{R}, & \forall c \in C, \forall p \in P, \\ \gamma_k^p \leq 0, & \forall k \in S, \forall p \in P, \\ \delta_j \leq 0, & \forall j \in J. \end{cases} \quad (7)$$

Noting that primal variables:

- x_{kj}^p are associated with dual constraints $\alpha_j^p + \gamma_k^p \leq ct_{kj}^p + h_j^p, \forall k \in S, \forall j \in F, \forall p \in P$;
- x_{jc}^p are associated with dual constraints $-\alpha_j^p + \beta_c^p \leq ct_{jc}^p, \forall j \in F, \forall c \in C, \forall p \in P$,

we can write complementary slackness conditions CS :

$$\text{CS} = \begin{cases} \gamma_k^p (s_k^p - \sum_{j \in F} x_{kj}^p) = 0, & \forall k \in S, \forall p \in P, \\ x_{kj}^p (ct_{kj}^p + h_j^p - \alpha_j^p - \gamma_k^p - r_j^p \delta_j) = 0, & \forall k \in S, \forall j \in F, \forall p \in P, \\ x_{jc}^p (ct_{jc}^p + \alpha_j^p - \beta_c^p) = 0, & \forall j \in F, \forall c \in C, \forall p \in P, \\ \delta_j (u_j - \sum_{p \in P} r_j^p \sum_{k \in S} x_{kj}^p) = 0, & \forall j \in F. \end{cases} \quad (8)$$

Let us consider the second constraint set in (8), i.e.,

$$x_{kj}^p (ct_{kj}^p + h_j^p - \alpha_j^p - \gamma_k^p - r_j^p \delta_j) = 0, \forall k \in S, \forall j \in F, \forall p \in P. \quad (9)$$

Let us assume that a positive flow x_{kj}^p travels from supplier k to facility j . This means that $ct_{kj}^p + h_j^p - \alpha_j^p - \gamma_k^p - r_j^p \delta_j = 0$, that is, $ct_{kj}^p + h_j^p - \gamma_k^p - r_j^p \delta_j = \alpha_j^p$. Since, by the dual feasibility $\gamma_k^p \leq 0$ and $\delta_j \leq 0$, we must have $\alpha_j^p \geq 0$. Moreover, when a positive quantity x_{kj}^p enters facility j , there must exist at least a client c such that $x_{jc}^p > 0$ which, in turn, by $x_{jc}^p (ct_{jc}^p + \alpha_j^p - \beta_c^p) = 0$ in (8), implies $ct_{jc}^p + \alpha_j^p - \beta_c^p = 0$. Now, since $\alpha_j^p \geq 0$ and $ct_{jc}^p > 0$ we have $\beta_c^p \geq ct_{jc}^p > 0$. If we linearize (9) by introducing binary variables $\tilde{q}_{kj}^p, \forall k \in S, \forall j \in F, \forall p \in P$, and a big- M parameter, as follows

$$\begin{aligned}
 ct_{kj}^p + h_j^p - \alpha_j^p - \gamma_k^p - r_j^p \delta_j &\leq M \tilde{q}_{kj}^p, & \forall k \in S, \forall j \in F, \forall p \in P, \\
 x_{k,j}^p &\leq M(1 - \tilde{q}_{kj}^p), & \forall k \in S, \forall j \in F, \forall p \in P, \end{aligned} \quad (10)$$

we can improve the formulation by adding the following constraints:

$$\alpha_j^p \geq -M \cdot \tilde{q}_{kj}^p, \forall k \in S, \forall j \in F, \forall p \in P. \quad (11)$$

In fact, when $\tilde{q}_{kj}^p = 1$, by constraints $x_{k,j}^p \leq M(1 - \tilde{q}_{kj}^p)$ and $x_{k,j}^p \geq 0$ we have $x_{k,j}^p = 0$, and (11) transforms into $\alpha_j^p \geq -M$, which is always verified; therefore, α_j^p remains a free variable as established in (7); on the contrary, when $x_{k,j}^p > 0$ we have $\tilde{q}_{kj}^p = 0$ and (11) becomes $\alpha_j^p \geq 0$ as explained above.

Moreover, if we linearize constraints $x_{j,c}^p(ct_{j,c}^p + \alpha_j^p - \beta_c^p) = 0, \forall j \in F, \forall c \in C, \forall p \in P$, by introducing binary variables $\tilde{q}_{j,c}^p, \forall j \in F, \forall c \in C, \forall p \in P$, and a big- M parameter, as follows

$$\begin{aligned} ct_{j,c}^p + \alpha_j^p - \beta_c^p &\leq M\tilde{q}_{j,c}^p, \quad \forall j \in F, \forall c \in C, \forall p \in P, \\ x_{j,c}^p &\leq M(1 - \tilde{q}_{j,c}^p), \quad \forall j \in F, \forall c \in C, \forall p \in P, \end{aligned} \quad (12)$$

we can further improve the model by adding the following additional constraints:

$$\beta_c^p \geq -M \cdot \tilde{q}_{j,c}^p + ct_{j,c}^p \cdot (1 - \tilde{q}_{j,c}^p), \forall c \in C, \forall j \in F, \forall p \in P. \quad (13)$$

In fact, when $\tilde{q}_{j,c}^p = 1$, by constraints $x_{j,c}^p \leq M(1 - \tilde{q}_{j,c}^p)$ and $x_{j,c}^p \geq 0$ we have $x_{j,c}^p = 0$, and (13) reduces to $\beta_c^p \geq -M$, which is always verified; therefore, β_c^p remains a free variable as established in (7); on the contrary, when $x_{j,c}^p > 0$ we have $\tilde{q}_{j,c}^p = 0$ and (13) becomes $\beta_c^p \geq ct_{j,c}^p$.

To fully linearize complementary slackness conditions in (8), we can introduce the following additional binary variables as follows.

- \bar{q}_k^p , associated with constraints $\gamma_k^p(s_k^p - \sum_{j \in F} x_{k,j}^p) = 0, \forall k \in S, \forall p \in P$;
- \bar{q}_j , associated with constraints $\delta_j(u_j - \sum_{p \in P} \sum_{j \in F} x_{k,j}^p) = 0, \forall j \in F$.

Hence, the overall linearized complementary conditions are:

$$\text{LCS} = \begin{cases} s_k^p - \sum_{j \in F} x_{k,j}^p \leq M\bar{q}_k^p, & \forall k \in S, \forall p \in P, \\ \gamma_k^p \geq M(\bar{q}_k^p - 1), & \forall k \in S, \forall p \in P, \\ ct_{k,j}^p + h_j^p - \alpha_j^p - \gamma_k^p - r_j^p \delta_j \leq M\bar{q}_{k,j}^p, & \forall k \in S, \forall j \in F, \forall p \in P, \\ x_{k,j}^p \leq M(1 - \tilde{q}_{k,j}^p), & \forall k \in S, \forall j \in F, \forall p \in P, \\ ct_{j,c}^p + \alpha_j^p - \beta_c^p \leq M\tilde{q}_{j,c}^p, & \forall j \in F, \forall c \in C, \forall p \in P, \\ x_{j,c}^p \leq M(1 - \tilde{q}_{j,c}^p), & \forall j \in F, \forall c \in C, \forall p \in P, \\ u_j - \sum_{p \in P} \sum_{j \in F} x_{k,j}^p \leq M\bar{q}_j, & \forall j \in F, \\ \delta_j \geq M(\bar{q}_j - 1), & \forall j \in F, \\ \bar{q}_k^p \in \{0, 1\}, & \forall k \in S, \forall p \in P, \\ \tilde{q}_{k,j}^p \in \{0, 1\}, & \forall k \in S, \forall j \in F, \forall p \in P, \\ \tilde{q}_{j,c}^p \in \{0, 1\}, & \forall c \in C, \forall j \in F, \forall p \in P, \\ \bar{q}_j \in \{0, 1\}, & \forall j \in J, \end{cases} \quad (14)$$

and, the overall single-level problem is

$$\begin{aligned} \min \sum_{j \in F} \sum_{p \in P} w_j^p + \sum_{p \in P} \sum_{(i,i) \in A} e_{i,i}^p x_{i,i}^p \\ \text{s.t. (2), (4), (6), (7), (11), (13), (14).} \end{aligned} \quad (15)$$

As proved in Kleinert et al. [25] a correct definition of the big- M can have beneficial effects on the computational time to solve the model. Therefore, in place of setting M to an arbitrarily large value, to attain the best possible bound, we defined M as the maximum value among $\{s_k^p, d_c^p, \frac{b_j}{ch_j}, ct_{j,c}^p, ct_{k,j}^p + h_j^p\}, \forall j \in F, \forall k \in S, \forall c \in C, \forall p \in P$.

It is known that the single-level problem (15) defines a so-called optimistic version of the bilevel program (5). Indeed, when the follower problem has multiple optimal solutions unless the follower

chooses the minimizer that allows the leader to optimize its objective function (semi-cooperative problem), there is a possible instability of the solution value of the single-level problem; in fact, there could be a gap between the latter (optimistic) solution value and the so-called pessimistic solution value, given by the optimal solution of the following problem, where $folloff$ is the optimal value of the follower objective function associated with the optimal solution of the single level problem, and \bar{u}_j , for every $j \in F$, are the capacities associated with such an optimistic solution:

$$\begin{aligned} \max \sum_{j \in F} \sum_{p \in P} w_j^p + \sum_{p \in P} \sum_{(i,i) \in A} e_{i,i}^p x_{i,i}^p \\ \text{s.t. } \sum_{k \in S} x_{k,j}^p - \sum_{c \in C} x_{j,c}^p = 0, & \quad \forall j \in F, \forall p \in P, \\ \sum_{j \in F} x_{j,c}^p = d_c^p, & \quad \forall c \in C, \forall p \in P, \\ \sum_{j \in F} x_{k,j}^p \leq s_k^p, & \quad \forall k \in S, \forall p \in P, \\ \sum_{p \in P} \sum_{j \in F} x_{k,j}^p \leq \bar{u}_j, & \quad \forall j \in F, \\ \sum_{p \in P} \sum_{(i,i) \in A} ct_{i,i}^p x_{i,i}^p + \sum_{p \in P} \sum_{j \in F} h_j^p \sum_{k \in S} x_{k,j}^p = folloff, & \\ x_{i,i}^p \geq 0, & \quad \forall (i,i) \in A, \forall p \in P. \end{aligned} \quad (16)$$

2.2. The definition of w_j^p and the resulting quadratic problem

We assume that emissions w_j^p associated with facility $j \in F$ and product $p \in P$ depend on both the investment z_j and the flow entering facility j . The reasons for this assumption are twofold.

- Investing in green technologies mainly means purchasing new machines with lower emissions, and therefore, the greater the investment at a site j , the lower the emissions per unit of product worked. In general, following studies conducted in the literature (see, e.g., Diaz et al. [13] and Luo et al. [29]) it is possible to derive the CO₂ reduction per worked part associated with each unit percentage of a given budget invested in green technology.
- The production machines in with each plant produce CO₂ for each product worked, and therefore the greater the inflow, the higher the emissions of site j ;

Hence, the function w_j^p can be defined as follows:

$$w_j^p = \phi_j^p (b_j - z_j) \sum_{k \in S} x_{k,j}^p.$$

where ϕ_j^p is a parameter that allows the transformation of the quantity $(b_j - z_j)$ from money to CO₂ emissions per unit of product p worked.

Now, we assume that z_j , i.e., the level of investment in facility $j \in F$, depends on the total amount of commodities (associated with all products $p \in P$) handled in facility $j \in F$, which means that

$$z_j = \zeta_j \sum_{p \in P} \sum_{k \in S} x_{k,j}^p,$$

where ζ_j is a parameter that allows the transformation of products into money.

The rationale behind this assumption is that the higher the number of overall products that will be processed in a plant j , the greater the investment in green technologies to reduce emissions. Therefore,

$$w_j^p = \phi_j^p \left(b_j - \zeta_j \sum_{p \in P} \sum_{k \in S} x_{k,j}^p \right) \sum_{k \in S} x_{k,j}^p.$$

The non-linear term w_j^p can be rewritten as follows:

Table 1
Parameter setting.

Parameter	Value
d_c^p	Uniform(50, 100) [units]
s_k^{p*}	Uniform(100, 120) [units]
ct_{ij}^p, h_j^p	Uniform(0.8, 1.2) [€/units]
e_{ij}^p	60/1000 [g/(kg km)] · Uniform(160, 240) [km] · 10[kg/units]
b_j^{**}	1200000 [€]
r_j^p	1 [dimensionless]
ch_j	100 [€/units]
ϕ	1 [g/€]
ζ	1 [€/units]

* Instances with 12 products and 20 facilities, with 17 products and 17 facilities, and with 15 products and 20 facilities have been generated using Uniform(200, 220). ** Instances with 15 products and 15 facilities have been generated with a budget ten times larger than that of the other instances.

$$w_j^p = \phi_j^p b_j \sum_{k \in S} x_{kj}^p - \phi_j^p \zeta_j \left(\sum_{p \in P} \sum_{k \in S} x_{kj}^p \right) \sum_{k \in S} x_{kj}^p.$$

2.3. The quadratic term in more detail: an example

Let $\bar{w}_j^p = \phi_j^p b_j \sum_{k \in S} x_{kj}^p$ and $\hat{w}_j^p = -\phi_j^p \zeta_j \left[\sum_{p \in P} \sum_{k \in S} x_{kj}^p \right] \sum_{k \in S} x_{kj}^p$, and let us see in more detail the quadratic term \hat{w}_j^p . For ease of presentation, let $\psi_j^p = \phi_j^p \zeta_j$, and consider a gadget network with $S = \{1, 2\}$, $F = \{3, 4\}$, $C = \{5, 6\}$, and $P = \{1, 2\}$. For each product and for each facility, \hat{w}_j^p can be written in the following way:

$$\begin{aligned} \hat{w}_3^1 &= -\psi_3^1 [x_{13}^1 + x_{23}^1 + x_{13}^2 + x_{23}^2] [x_{13}^1 + x_{23}^1] \\ &= -\psi_3^1 \left[(x_{13}^1)^2 + (x_{23}^1)^2 + x_{13}^1 x_{23}^1 + x_{13}^1 x_{23}^2 + x_{13}^2 x_{13}^1 + x_{23}^2 x_{13}^1 + x_{13}^1 x_{23}^2 + x_{23}^2 x_{23}^1 \right] \\ &= -\psi_3^1 \left[(x_{13}^1)^2 + (x_{23}^1)^2 + 2x_{13}^1 x_{23}^1 + x_{13}^1 x_{23}^2 + x_{23}^2 x_{13}^1 + x_{13}^2 x_{23}^1 + x_{23}^2 x_{23}^1 \right], \end{aligned}$$

$$\begin{aligned} \hat{w}_3^2 &= -\psi_3^2 [x_{13}^2 + x_{23}^2 + x_{13}^1 + x_{23}^1] [x_{13}^2 + x_{23}^2] \\ &= -\psi_3^2 \left[(x_{13}^2)^2 + (x_{23}^2)^2 + 2x_{13}^2 x_{23}^2 + x_{13}^2 x_{23}^1 + x_{13}^1 x_{23}^2 + x_{23}^1 x_{13}^2 + x_{23}^2 x_{23}^1 \right], \end{aligned}$$

$$\begin{aligned} \hat{w}_4^1 &= -\psi_4^1 [x_{14}^1 + x_{24}^1 + x_{14}^2 + x_{24}^2] [x_{14}^1 + x_{24}^1] \\ &= -\psi_4^1 \left[(x_{14}^1)^2 + (x_{24}^1)^2 + 2x_{14}^1 x_{24}^1 + x_{14}^1 x_{24}^2 + x_{14}^2 x_{14}^1 + x_{24}^2 x_{14}^1 + x_{24}^1 x_{24}^2 \right], \end{aligned}$$

$$\begin{aligned} \hat{w}_4^2 &= -\psi_4^2 [x_{14}^2 + x_{24}^2 + x_{14}^1 + x_{24}^1] [x_{14}^2 + x_{24}^2] \\ &= -\psi_4^2 \left[(x_{14}^2)^2 + (x_{24}^2)^2 + 2x_{14}^2 x_{24}^2 + x_{14}^2 x_{24}^1 + x_{14}^1 x_{24}^2 + x_{24}^1 x_{14}^2 + x_{24}^2 x_{24}^1 \right]. \end{aligned}$$

We can now rewrite the term \hat{w}_j^p in quadratic form $\mathbf{x}^T \mathbf{H} \mathbf{x}$, where

$$\mathbf{x}^T = (x_{13}^1, x_{23}^1, x_{13}^2, x_{23}^2, x_{14}^1, x_{24}^1, x_{14}^2, x_{24}^2)$$

and

$$\mathbf{H} = \begin{pmatrix} \Psi_1 & \mathbf{0} \\ \mathbf{0} & \Psi_2 \end{pmatrix}$$

where

$$\mathbf{0} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

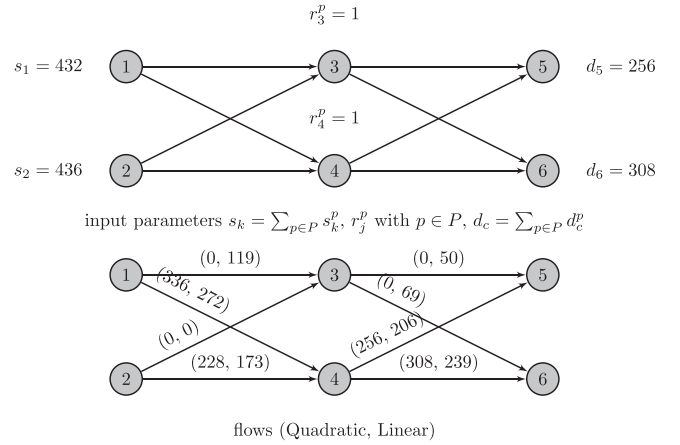


Fig. 2. Example network with $|S| = 2$, $|F| = 2$, and $|C| = 2$ and optimal flows for the quadratic and linear model.

$$\Psi_1 = \begin{pmatrix} -\psi_3^1 & -\psi_3^1 & -\frac{1}{2}(\psi_3^1 + \psi_3^2) & -\frac{1}{2}(\psi_3^1 + \psi_3^2) \\ -\psi_3^1 & -\psi_3^1 & -\frac{1}{2}(\psi_3^1 + \psi_3^2) & -\frac{1}{2}(\psi_3^1 + \psi_3^2) \\ -\frac{1}{2}(\psi_3^1 + \psi_3^2) & -\frac{1}{2}(\psi_3^1 + \psi_3^2) & -\psi_3^2 & -\psi_3^2 \\ -\frac{1}{2}(\psi_3^1 + \psi_3^2) & -\frac{1}{2}(\psi_3^1 + \psi_3^2) & -\psi_3^2 & -\psi_3^2 \end{pmatrix}$$

$$\Psi_2 = \begin{pmatrix} -\psi_4^1 & -\psi_4^1 & -\frac{1}{2}(\psi_4^1 + \psi_4^2) & -\frac{1}{2}(\psi_4^1 + \psi_4^2) \\ -\psi_4^1 & -\psi_4^1 & -\frac{1}{2}(\psi_4^1 + \psi_4^2) & -\frac{1}{2}(\psi_4^1 + \psi_4^2) \\ -\frac{1}{2}(\psi_4^1 + \psi_4^2) & -\frac{1}{2}(\psi_4^1 + \psi_4^2) & -\psi_4^2 & -\psi_4^2 \\ -\frac{1}{2}(\psi_4^1 + \psi_4^2) & -\frac{1}{2}(\psi_4^1 + \psi_4^2) & -\psi_4^2 & -\psi_4^2 \end{pmatrix}$$

3. Computational analysis

In this section, we report our experimental study. Instances have been generated and classified by size as small and large. In small-size instances, the number of products ranges from 2 to 5 and there are from 2 to 5 nodes for each supply chain layer. In large-size instances, the number of products varies from 5 to 15 and the number of nodes for each supply chain layer ranges from 7 to 20. Parameters used are reported in Table 1.

In the experimentation, we first used the optimistic version of the bilevel formulation (15). Notwithstanding, for the sake of completeness, in Section 3.5 we tested the stability of these solutions using the pessimistic version of the problem (16). Indeed, the optimistic version of the problem gives the information on the solution providing the smallest objective value of the leader in a hierarchical decision scenario, enabling, therefore, the worst-case analysis provided by the pessimistic version of the problem which strongly relies on the information tunneled by the related optimistic version.

All the models have been coded using the PYOMO Python library and solved with the solver CPLEX™ release 12.10. The latter has the specific functionality (which must be enabled) to solve problems containing non-convexity. This flag allowed us to solve all of the generated instances. The machine used for the experiments is equipped with an Intel (R) Xeon (R) Gold 6136 CPU @ 3.00 GHz processor with 48 cores and 256 GB RAM. A time limit was set to 7200 s

Table 2
Instance with $|P| = 4$, $|S| = 2$, $|F| = 2$, and $|C| = 2$; values of the z variables.

j	z (quadratic)	z (linear)
3	0	119
4	564	445

Table 3
Instance with $|P| = 4$, $|S| = 2$, $|F| = 2$, and $|C| = 2$; value of the x variables entering the nodes in F .

p	k	j	x (quadratic)	x (linear)
1	1	3	0	0
2	1	3	0	50
3	1	3	0	0
4	1	3	0	69
1	2	3	0	0
2	2	3	0	0
3	2	3	0	0
4	2	3	0	0
1	1	4	118	118
2	1	4	103	53
3	1	4	101	101
4	1	4	14	0
1	2	4	73	73
2	2	4	0	0
3	2	4	41	41
4	2	4	114	59

3.1. Quadratic vs linear objective function

The performance of (15) is compared to the performance of the same model where the quadratic objective is replaced with a linear function where w_j^p is defined as

$$w_j^p = \phi_j^p \left[b_j - \zeta_j \sum_{p \in P} \sum_{k \in S} x_{kj}^p \right].$$

The main objective of the experiments is to measure the CO₂ emissions performed by the two models, quadratic and linear, identified by letters Q and L, respectively.

Before presenting extensive computational results, to show how the network can be settled differently if emissions are modeled linearly ($w_j^p = \bar{w}_j^p$) or quadratically ($w_j^p = \bar{w}_j^p + \hat{w}_j^p$), we consider a gadget network with $|P| = 4$, $|S| = 2$, $|F| = 2$, and $|C| = 2$. Fig. 2 shows the network: in the upper part, we report the setting of the parameters in terms of the aggregate capacity for each supplier node, the handling capacity of the facilities, and the aggregated demand of customers. Instead, the lower part of the figure reports, for each arc, the optimal flows obtained by the quadratic model and the linear model, respectively, solved at the optimum by CPLEX.

The different solutions are associated with different values of the variable z , which are detailed in Table 2, while the flow entering facilities 3 and 4 is reported in Table 3. It is easy to note how the quadratic model concentrates flows in a single node, whereas the solution of the linear model is more sparse. The rationale is that the linear model tends not to take into account the effect of the accumulation of operations; conversely, the quadratic model considers this phenomenon.

3.2. Computational results on synthetic instances

3.2.1. Small balanced instances

These instances are classified by $|P|$, the number of products, $|S|$, the number of suppliers, $|F|$, the number of facilities, $|C|$, the number of customers, and are balanced meaning that $|S| = |F| = |C|$.

Table 4, in column Obj, reports the results obtained by (15) implemented with its (native) quadratic objective (see letter Q in column Type) and the variant of (15) implemented with the linear objective (see

Table 4
Results for small instances.

(P , S , F , C)	Type	Obj	Time (s)	ObjValQ	ObjValL	ΔQ	ΔL
(2,2,2,2)	Q	352,781,186.1	0.0	352,781,186.1	4867,034.1	0.0	
(2,2,2,2)	L	4867,034.1	0.1	352,781,186.1	4867,034.1		0.0
(2,3,3,3)	Q	523,102,141.7	0.1	523,102,141.7	7291,365.7	-120324.3	
(2,3,3,3)	L	7289,764.0	0.1	523,222,466.0	7289,764.0		-1601.7
(2,4,4,4)	Q	676,613,251.3	1.0	676,613,251.3	9730,219.3	-216276.5	
(2,4,4,4)	L	9720,779.9	0.1	676,829,527.9	9720,779.9		-9439.5
(2,5,5,5)	Q	881,642,499.3	0.3	881,642,499.3	12,181,254.3	-372980.4	
(2,5,5,5)	L	12,150,672.7	0.1	882,015,479.7	12,150,672.7		-30581.6
(3,2,2,2)	Q	523,108,608.7	0.1	523,108,608.7	7297,396.7	-89199.4	
(3,2,2,2)	L	7292,196.2	0.1	523,197,808.2	7292,196.2		-5200.6
(3,3,3,3)	Q	761,748,316.4	0.3	761,748,316.4	10,949,636.4	-246608.3	
(3,3,3,3)	L	10,935,688.7	0.1	761,994,924.7	10,935,688.7		-13947.7
(3,4,4,4)	Q	1072,206,447.6	0.5	1072,206,447.6	14,603,001.6	-558285.1	
(3,4,4,4)	L	14,587,008.8	0.1	1072,764,732.8	14,587,008.8		-15992.9
(3,5,5,5)	Q	1316,638,712.5	7.1	1316,638,712.5	18,241,022.4	-875695.3	
(3,5,5,5)	L	18,220,719.8	0.1	1317,514,407.8	18,220,719.8		-20302.6
(4,2,2,2)	Q	676,603,982.2	0.1	676,603,982.2	9719,822.2	-104149.0	
(4,2,2,2)	L	9718,061.3	0.1	676,708,131.3	9718,061.3		-1760.9
(4,3,3,3)	Q	1072,225,909.9	0.1	1072,225,909.9	14,621,569.9	-471459.4	
(4,3,3,3)	L	14,595,877.3	0.1	1072,697,369.3	14,595,877.3		-25692.6
(4,4,4,4)	Q	1390,923,356.8	1.1	1390,923,356.8	19,464,316.8	-985855.3	
(4,4,4,4)	L	19,443,314.1	0.2	1391,909,212.1	19,443,314.1		-21002.7
(4,5,5,5)	Q	1751,424,845.0	1.9	1751,424,845.0	24,353,522.0	-1584454.4	
(4,5,5,5)	L	24,295,914.4	0.2	1753,009,299.4	24,295,914.4		-57607.6
(5,2,2,2)	Q	881,636,318.8	0.1	881,636,318.8	12,172,868.8	-249517.4	
(5,2,2,2)	L	12,164,598.3	0.1	881,885,836.3	12,164,598.3		-8270.6
(5,3,3,3)	Q	1316,655,416.6	0.9	1316,655,416.6	18,255,530.6	-725590.7	
(5,3,3,3)	L	18,228,943.3	0.1	1317,381,007.3	18,228,943.3		-26587.3
(5,4,4,4)	Q	1751,404,790.6	2.5	1751,404,790.6	24,332,006.6	-1545705.7	
(5,4,4,4)	L	24,297,564.3	0.2	1752,950,496.3	24,297,564.3		-34442.3
(5,5,5,5)	Q	2228,976,862.8	0.6	2228,976,862.8	30,427,162.8	-2528738.5	
(5,5,5,5)	L	30,375,363.2	0.2	2231,505,601.2	30,375,363.2		-51799.5

Table 5
Results for large instances.

(P , S , F , C)	Type	Obj	Time (s)	Gap	ObjValQ	ObjValL	ΔQ	ΔL
(5,10,10,10)	Q	4340,083,501.8	0.7	0.00	4340,083,501.8	60,820,495.8	-11,597,913.0	
(5,10,10,10)	L	60,707,988.9	0.5	0.00	4351,681,414.9	60,707,988.9		-112507.0
(5,12,12,12)	Q	5218,762,283.6	1.0	0.00	5218,762,283.6	72,984,959.6	-17,067,473.1	
(5,12,12,12)	L	72,849,730.5	0.7	0.00	5235,829,756.7	72,849,730.5		-135229.1
(5,15,15,15)	Q	6590,046,838.0	2.3	0.00	6590,046,838.0	91,245,514.0	-28,129,489.6	
(5,15,15,15)	L	91,063,827.6	0.7	0.00	6618,176,327.6	91,063,827.6		-181686.5
(5,17,17,17)	Q	7401,813,793.7	2.9	0.00	7401,813,793.7	103,410,399.7	-35,522,545.6	
(5,17,17,17)	L	103,190,049.2	0.9	0.00	7437,336,339.2	103,190,049.2		-220350.4
(5,20,20,20)	Q	8652,648,298.7	3.6	0.00	8652,648,298.7	12,161,8042.7	-49,344,288.2	
(5,20,20,20)	L	121,386,274.9	1.6	0.00	8701,992,586.9	121,386,274.9		-231767.7
(7,10,10,10)	Q	6089,236,214.2	1.1	0.00	6089,236,214.2	85,159,574.2	-22,779,101.5	
(7,10,10,10)	L	84,986,721.7	0.8	0.00	6112,015,315.7	84,986,721.7		-172852.5
(7,12,12,12)	Q	7337,664,224.4	2.2	0.00	7337,664,224.4	102,182,234.4	-34,165,690.3	
(7,12,12,12)	L	101,984,032.7	1.3	0.00	7371,829,914.7	101,984,032.7		-198201.7
(7,15,15,15)	Q	9159,979,116.5	3.3	0.00	9159,979,116.5	127,723,110.5	-54,281,071.6	
(7,15,15,15)	L	127,467,228.2	1.0	0.00	9214,260,188.2	127,467,228.2		-255882.3
(7,17,17,17)	Q	10,451,520,968.0	5.0	0.00	10,451,520,968.0	144,807,548.0	-71,860,443.1	
(7,17,17,17)	L	144,474,169.1	1.2	0.00	10,523,381,411.1	144,474,169.1		-333378.9
(7,20,20,20)	Q	12,336,508,061.7	24.0	0.00	12,336,508,061.7	170,330,909.7	-101,322,449.4	
(7,20,20,20)	L	169,964,645.2	3.4	0.00	12,437,830,511.1	169,964,645.2		-366264.5
(10,10,10,10)	Q	8652,658,526.8	1.9	0.00	8652,658,526.8	121,592,005.8	-46,727,098.9	
(10,10,10,10)	L	121,385,546.6	1.0	0.00	8699,385,625.8	121,385,546.6		-206459.2
(10,12,12,12)	Q	10,525,976,043.8	3.1	0.00	10,525,976,043.8	145,944,918.8	-71,030,907.5	
(10,12,12,12)	L	145,672,840.3	1.2	0.00	10,597,006,951.3	145,672,840.3		-272078.5
(10,15,15,15)	Q	13,214,650,460.5	9.1	0.00	13,214,650,460.5	182,438,096.4	-114,070,436.1	
(10,15,15,15)	L	182,095,013.6	1.9	0.00	13,328,720,896.5	182,095,013.6		-343082.9
(10,17,17,17)	Q	15,014,724,375.5	19.9	0.19	15,014,724,375.5	206,718,114.0	-131,038,116.5	
(10,17,17,17)	L	206,365,682.0	3.7	0.00	15,145,762,492.0	206,365,682.0		-352432.0
(10,20,20,20)	Q	17,620,733,690.1	11.4	0.11	17,620,733,690.1	243,102,785.5	-137,916,775.0	
(10,20,20,20)	L	242,760,037.2	4.4	0.00	17,758,650,465.1	242,760,037.2		-342748.3
(12,10,10,10)	Q	10,525,999,501.2	1.9	0.00	10,525,999,501.2	145,950,706.2	-69,441,103.4	
(12,10,10,10)	L	145,673,635.6	1.1	0.00	10,595,440,604.6	145,673,635.6		-277,070.6
(12,12,12,12)	Q	12,670,215,387.5	5.2	0.00	12,670,215,387.5	175,131,374.7	-103,111,844.3	
(12,12,12,12)	L	174,800,534.8	1.1	0.00	12,773,327,231.8	174,800,534.8		-330,839.9
(12,15,15,15)	Q	15,837,767,004.9	15.6	0.11	15,837,767,004.9	218,824,787.0	-130,381,803.0	
(12,15,15,15)	L	218,474,594.8	2.1	0.00	15,968,148,807.9	218,474,594.8		-350,192.3
(12,17,17,17)	Q	17,944,353,277.9	41.2	0.18	17,944,353,277.9	247,947,055.7	-136,375,106.1	
(12,17,17,17)	L	247,592,556.8	2.7	0.00	18,080,728,383.9	247,592,556.8		-354,498.9
(12,20,20,20)	Q	38,842,781,634.0	12.1	0.00	38,842,781,634.0	531,736,862.0	-299,675,779.2	
(12,20,20,20)	L	531,271,163.0	3.8	0.00	39,142,457,413.3	531,271,163.0		-465,699.1
(15,10,10,10)	Q	13,214,680,231.7	3.0	0.00	13,214,680,231.7	182,412,305.7	-110,622,931.3	
(15,10,10,10)	L	182,069,187.1	1.3	0.00	13,325,303,163.1	182,069,187.1		-343,118.6
(15,12,12,12)	Q	15,837,766,942.8	12.9	0.10	15,837,766,942.8	218,785,665.4	-127,788,485.8	
(15,12,12,12)	L	218,452,288.6	1.5	0.00	15,965,555,428.6	218,452,288.6		-333,376.8
(15,15,15,15)	Q	1995,14,627,516.1	17.2	0.00	199,514,627,516.1	2703,566,981.7	-256,924,281.7	
(15,15,15,15)	L	2703,042,401.6	3.7	0.00	199,771,551,797.8	2703,042,401.6		-524,580.1
(15,17,17,17)	Q	41,272,408,237.0	13.1	0.00	41,272,408,237.0	564,928,663.0	-334,793,660.3	
(15,17,17,17)	L	564,437,683.3	2.4	0.00	41,607,201,897.2	564,437,683.3		-490,979.7
(15,20,20,20)	Q	48,781,534,433.3	11.7	0.03	48,781,534,433.3	664,627,503.0	-447,174,187.7	
(15,20,20,20)	L	664,059,730.5	3.4	0.00	49,228,708,621.0	664,059,730.5		-567,772.5

letter L in column Type). By setting the minimum optimality gap to 0.2%, all the instances have been solved in a limited computational time.

Column ObjValQ reports the value of the quadratic objective function computed on the optimal solution found by (15) implemented with (i) its original quadratic function (row Q) and (ii) the modified linear function (row L). Column ObjValL, instead, reports the value of the linear objective function computed on the optimal solution found by (15) implemented with (i) its original quadratic function (row Q) and (ii) the modified linear function (row L).

Column ΔQ reported on the Q row of each instance, lists the difference between the ObjValQ values of the Q and the L rows of each instance. In contrast, ΔL , reported on the L row of each instance, reports the difference between the ObjValL values of the Q and the L rows of each instance. A negative ΔQ means that the solution of our model implemented with its quadratic function accounts for lower CO₂ emissions if this is evaluated by the quadratic function. All ΔQ and ΔL values are negative (but the smallest instance that has $\Delta Q = \Delta L = 0$) meaning that our model defined with its native quadratic function performs

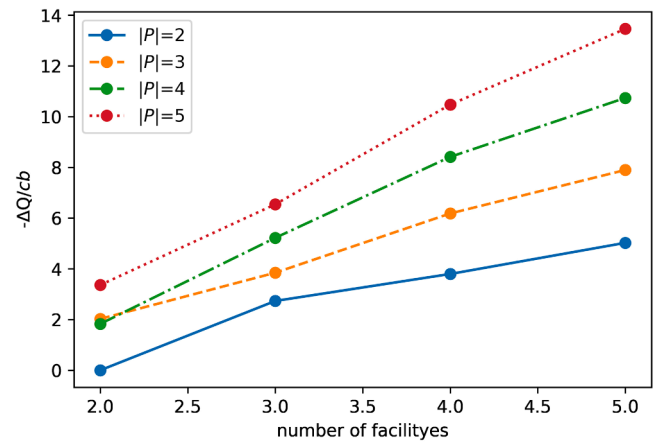


Fig. 3. The ratio $-\Delta Q$ over the consumed budget (cb) for different numbers of products (small instances).

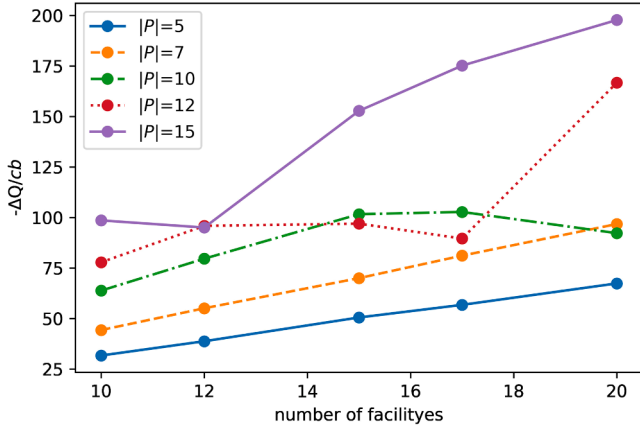


Fig. 4. The ratio $-\Delta Q$ over the consumed budget (cb) for different numbers of products (large instances).

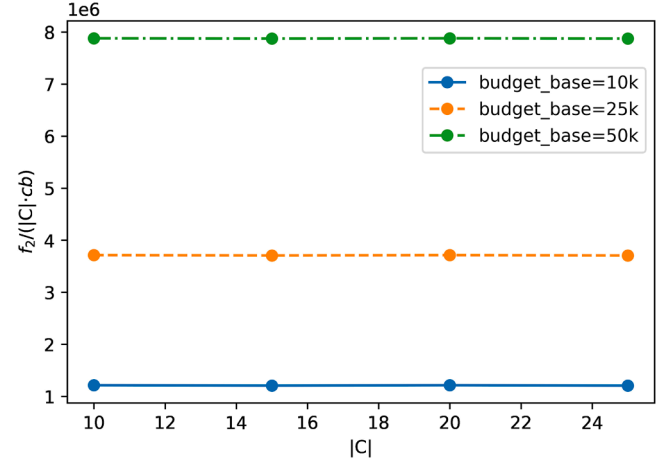


Fig. 6. The ratio $\frac{f_2}{|C| \cdot cb}$ for different numbers of clients and budget amounts (unbalanced instances, $|F| = 3$).

Table 6
Parameter setting for unbalanced instances.

Parameters	Facility Analysis	Customer Analysis
$ P $	5	5
$ F $	{10, 15, 20, 25}	3
$ C $	3	{10, 15, 20, 25}
d_e^p	uniform(50, 100) [units]	uniform(50, 100) [units]
s_k^p	uniform(50, 200) [units]	uniform(50, 200) · $ C / F $ [units]
u_j	uniform(100, 120) [units]	uniform(100, 120) [units]
$ct_{i,l}^p$	uniform(0.5, 1.5) [€/units]	uniform(0.5, 1.5) [€/units]
ht_j^p	uniform(0.5, 1.5) [€/units]	uniform(0.5, 1.5) [€/units]
e_{li}^p	uniform(100, 300) · 600/1000 [g/units]	uniform(100, 300) · 600/1000 [g/units]
budget_base	{10000, 25000, 50000} [dimensionless]	{10000, 25000, 50000} [dimensionless]
b_j	budget_base · (120/ F) [€]	budget_base · (120/ F) · (C / F) [€]

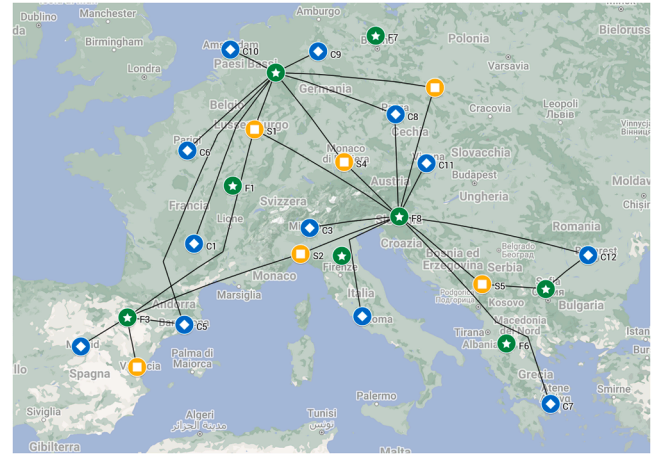


Fig. 7. Active flows of the green supply chain based on the realistic case. Rectangle placeholders represent suppliers, star placeholders represent facilities, and diamond placeholders represent customers.

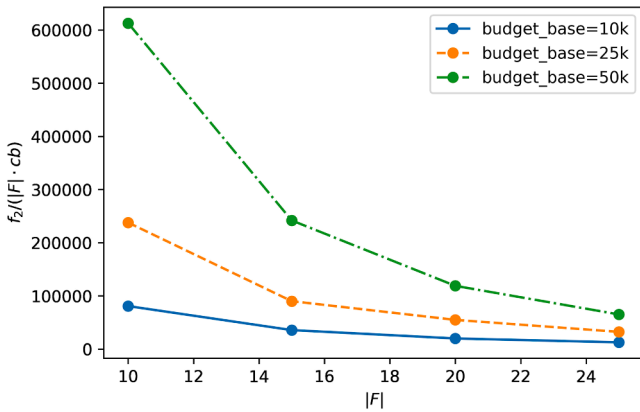


Fig. 5. The ratio $\frac{f_2}{|F| \cdot cb}$ for different numbers of facilities and budget amounts (unbalanced instances, $|C| = 3$).

better than its linear variant; note that when $|P|$ and/or the number of supply chain nodes increases, the underestimation of the linear model tends to be significant.

3.2.2. Large balanced instances

In Tables 5, we report results on large instances with number of products $|P| = 5, 7, 10, 12, 15$. Only in 6 out of 50 cases, we had a positive optimality gap, lower than 0.2% (see column Gap); in all the other cases, instances were solved to the optimum. The linear model was

always solved to the optimum within a very limited computing time (lower than that of the quadratic case) for all the instances. The behavior of the proposed model is the same as the one observed in Table 4. In this case, the numbers say that the difference in the accounted CO₂ emissions is much greater with much more remarkable growing patterns.

To show the robust behavior of the quadratic model compared to the linear one, in Fig. 3 (small instances) and in Fig. 4 (large instances), we plot the average difference of the ratio $\frac{-\Delta Q}{\text{consumed_budget}}$ for different numbers of products and facilities, where $\text{consumed_budget} = \sum_{j \in F} [z_j + ch_j \mu_j]$. By the charts, it appears that the improvements ($-\Delta Q$) in terms of lower emissions of the quadratic model as compared to the linear one tend to increase for increasing number of facilities.

3.3. Unbalanced instances

A further experimental test has been conducted on unbalanced instances, i.e., instances where the number of suppliers is different from the number of facilities and customers. The setting for this test is detailed in Table 6.

The first experimentation is reported in Fig. 5 showing the results obtained for different numbers of facilities and budget amounts. It can be seen that, as the number of facilities grows, the CO₂ emissions divided by the number of facilities times the consumed budget decrease. Another

Table 7

Parameter setting for the realistic case, $|S| = 6$, $|F| = 8$, $|C| = 12$, $|P| = 1$.

Parameter	Value
d_c^p	36000 [units]
s_k^p	45000 [units]
$c_{i,i}^p$	0.1·dist _{i,i} [€/units]
h_j^p	Uniform(0.8, 1.2) [€/units]
$e_{i,i}^p$	0.1·dist _{i,i} [g/units]
b_j	1, 800, 000 [€]
r_j^p	1 [dimensionless]
ch_j	1 [€/units]
ϕ	$1.167 \cdot 10^{-5}$ [g/€]
ζ	1 [€/units]

Table 8

Positive flows ($x_{i,i}^p$, $p = 1$) in the case study supply networks.

from	to	i	i'	$x_{i,i}$
S1	F2	1	8	6244
S1	F3	1	9	453
S1	F8	1	14	39
S2	F3	2	9	936
S2	F8	2	14	6521
S3	F3	3	9	3541
S4	F2	4	8	3963
S4	F8	4	14	1917
S5	F5	5	11	1070
S5	F8	5	14	5007
S6	F2	6	8	4794
S6	F8	6	14	1516
F2	C1	8	15	3000
F2	C5	8	19	1070
F2	C6	8	20	3000
F2	C8	8	22	1930
F2	C9	8	23	3000
F2	C10	8	24	3000
F3	C4	9	18	3000
F3	C5	9	19	1930
F5	C12	11	26	1070
F8	C2	14	16	3000
F8	C3	14	17	3000
F8	C7	14	21	3000
F8	C8	14	22	1070
F8	C11	14	25	3000
F8	C12	14	26	1930

fact to be noted is that this behavior is similar also if the value on the Y-axis is not divided by the number of facilities since when the number of facilities grows, the model can more effectively select the most appropriate facilities where investing to decrease the emissions. Furthermore, when the available budget grows, this happens because the parameter b_j is in the objective function. In real applications, this may require a fine-tuning of the parameters of the objective function ϕ , ch , and ζ .

A further test has been carried out to verify the model behavior on unbalanced instances with a growing number of customers. The results are detailed in Fig. 6. Even in this case, different plots are reported for different budget amounts, the emissions, divided by the number of customers times the consumed budget, are drawn when the number of customers in the instance increases which means that the quadratic model performs better than the linear one. The interesting insight is that the plotted values are stationary over an increasing number of customers when the other settings of the network are kept fixed.

3.4. A case study

We adapted the case described in Caramia and Stecca [8] and Wang et al. [40] to show the behavior of the proposed model in a realistic

Table 9

Investment levels for the case study.

j	z_j
7	0.00
8	15000.00
9	4929.67
10	0.00
11	1070.33
12	0.00
13	0.00
14	15000.00

Table 10

Stability results.

($ P $, $ S $, $ F $, $ C $)	Optimistic	Pessimistic	Time (s)	Δ
(2,2,2,2)	352,781,186.1	352,784,464.6	0.1	0.00
(2,3,3,3)	523,102,141.7	523,108,086.5	0.0	0.00
(2,4,4,4)	676,613,251.3	676,618,655.4	0.0	0.00
(2,5,5,5)	881,642,499.3	881,646,908.2	0.0	0.00
(3,2,2,2)	523,108,608.7	523,110,539.9	0.0	0.00
(3,3,3,3)	761,748,316.4	761,754,265.9	0.0	0.00
(3,4,4,4)	1072,206,447.6	1072,214,904.0	0.0	0.00
(3,5,5,5)	1316,638,712.5	1316,654,331.4	0.0	0.00
(4,2,2,2)	676,603,982.2	676,605,376.9	0.0	0.00
(4,3,3,3)	1072,225,909.9	1072,229,170.5	0.0	0.00
(4,4,4,4)	1390,923,356.8	1390,931,162.4	0.0	0.00
(4,5,5,5)	1751,424,845.0	1751,434,509.8	0.1	0.00
(5,2,2,2)	881,636,318.8	881,640,385.1	0.1	0.00
(5,3,3,3)	1316,655,416.6	1316,667,724.0	0.1	0.00
(5,4,4,4)	1751,404,790.6	1751,425,240.4	0.1	0.00
(5,5,5,5)	2228,976,862.8	2228,997,825.7	0.1	0.00
(5,10,10,10)	4340,083,501.8	4340,137,192.5	0.2	0.00
(5,12,12,12)	5218,762,283.6	5218,827,028.6	0.2	0.00
(5,15,15,15)	6590,046,838.0	6590,126,735.7	0.3	0.00
(5,17,17,17)	7401,813,793.7	7401,905,824.9	0.6	0.00
(5,20,20,20)	8652,648,298.7	8652,764,805.3	0.7	0.00
(7,10,10,10)	6089,236,214.2	6089,312,414.2	0.2	0.00
(7,12,12,12)	7337,664,224.4	7337,751,100.5	0.3	0.00
(7,15,15,15)	9159,979,116.5	9160,089,066.3	0.6	0.00
(7,17,17,17)	10,451,520,968.0	10,451,652,254.3	0.8	0.00
(7,20,20,20)	12,336,508,061.7	12,336,675,281.0	1.2	0.00
(10,10,10,10)	8652,658,526.8	8652,755,101.6	0.4	0.00
(10,12,12,12)	10,525,976,043.8	10,526,109,571.3	0.6	0.00
(10,15,15,15)	13,214,650,460.5	13,214,812,137.4	1.0	0.00
(10,17,17,17)	15,014,724,375.5	15,015,006,307.2	1.4	0.00
(10,20,20,20)	17,620,733,690.1	17,621,231,814.2	2.5	0.00
(12,10,10,10)	10,525,999,501.2	10,526,118,874.8	0.5	0.00
(12,12,12,12)	12,670,215,387.5	12,670,362,990.7	0.8	0.00
(12,15,15,15)	15,837,767,004.9	15,838,144,396.2	1.4	0.00
(12,17,17,17)	17,944,353,277.9	17,944,884,579.6	2.2	0.00
(12,20,20,20)	38,842,781,634.0	38,843,298,235.6	4.2	0.00
(15,10,10,10)	13,214,680,231.7	13,214,826,874.2	0.7	0.00
(15,12,12,12)	15,837,766,942.8	15,838,127,725.2	1.2	0.00
(15,15,15,15)	199,514,627,516.1	199,514,885,344.7	2.8	0.00
(15,17,17,17)	41,272,408,237.0	41,273,000,019.1	3.9	0.00
(15,20,20,20)	48,781,534,433.3	48,782,296,210.2	6.5	0.00

scenario. In the latter, the supply network is formed of $|S| = 6$ suppliers, $|F| = 8$ facilities, and $|C| = 12$ customers, and $|P| = 1$ products (Fig. 7 depicts the nodes of the supply network). The distances $\text{dist}_{i,i}$ between pairs of nodes (i, i') are estimated based on the real location of the nodes in the map. The parameters are set as detailed in Table 7.

In the case study instance, the solver was able to find a solution with a gap of 4.2% after 600 s of running time. The best solution found has a leader objective function equal to $9.2388 \cdot 10^7$ (we recall that this value is the square of the emissions). In this condition, the follower can reach a minimum value of the overall supply chain cost equal to 3, 448, 685.01. The results are detailed in Tables 8 and 9. Fig. 7 depicts active flows in to optimal solution of the green supply chain. The flow appears balanced among facilities. 4 out of 8 facilities are activated and they are sourced by all 6 suppliers. We noticed that, with the defined settings, the green

supply chain tends to concentrate production on a few facilities. By removing the facility capacity constraints, the production and the green investments will be concentrated in only one facility.

3.5. The solution stability test

To verify the bilevel model stability, the optimal solution values of (16) have been tested against the previously presented (optimistic) solution values of the balanced instances. The results are detailed in Table 10. For each instance, we show the values of the optimistic and pessimistic solutions, the computational time to solve the pessimistic problem, and, to ease the readability of the results, the value Δ which represents the difference between the pessimistic solution value and the optimistic solution value, divided by the pessimistic solution value. The results, which show a negligible difference between the two solution values, indicate that the model is stable.

4. Conclusions

Green Supply Chain Management requires coordinated decisions between the strategic and operational layers to achieve strict green goals. In this paper, we proposed a new mathematical programming model for the minimization of CO₂ emissions, in a three-layered supply chain, where investments in facility installation must be shared with investments in green practices, and where demand must be satisfied by operations. The problem has been modeled as a bilevel programming problem. A theoretical framework is also presented to strengthen the formulation of the single-level reformulation of the problem. The leader objective function models CO₂ emissions in a non-convex quadratic form. A comparison has been conducted with the same model, in which the leader objective is formulated as a linear function. The computational analysis shows the underestimation of the emissions performed by the linear model compared to the quadratic one. The quadratic model can exploit solutions with a different flow of goods, resulting in a lower emission level and more efficient budget expenditure in green practices. A further study has been devoted to analyzing the effect of variations in budget, customers, and facilities, and to verifying the stability of the model, by solving the pessimistic version of the latter. Since in the current literature, little or no attention to the nonlinear treatment of carbon emissions, and no consideration of investments to neutralize the latter, especially in a bilevel programming setting has been devoted we believe that the proposed model represents a step toward filling this gap. As for future work, we plan to develop extensions of the proposed model considering different measures of sustainability and nonlinear definitions of emissions. Moreover, the possible development of heuristics or metaheuristics for the bilevel program can be object of future work. This may be worthwhile especially when large hard instances have to be solved. Indeed, in the latter scenarios, it appears to be viable to implement either (i) a so-called nested approach where the metaheuristic first finds leader solutions and then, for each of them, solves the follower problem, or (ii) a standard metaheuristic to solve the proposed single-level reformulation in place of using an off-the-shelf solver to find optimal solutions (see, e.g., Camacho-Vallejo et al. [6]).

CRedit authorship contribution statement

Massimiliano Caramia: Writing – original draft, Validation, Methodology, Conceptualization. **Giuseppe Stecca:** Writing – original draft, Validation, Software, Methodology, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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