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Joint Design and Pricing Problem for Symbiotic Bioethanol Supply Chain Network: Model and Resolution Approach☆

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ABSTRACT

To fight climate change, the Province of Quebec, Canada, has set targets to reduce greenhouse gas emissions by reducing fossil fuel consumption and integrating biofuel content into gasoline and diesel fuel. Motivated by a real-world case study, this paper presents a novel distributed decision model for designing a symbiotic supply chain network and supporting pricing decisions. A distributed decision-making problem is formulated as a game theoretic approach considering a Stackelberg–Nash equilibrium. A novel mathematical model is proposed to support the decisions of four actors: corn farms, processing depots, pig farms, and biorefineries. In addition to the configuration of a biofuel-based industrial symbiosis, the model offers the possibility of setting purchase prices and supply levels for biomass (corn stover supplied by farms), as well as determining sales prices and production levels for the main product (the cellulosic sugar used for the bioethanol production) and a coproduct (pig feed sold to pig farmers). A three-step optimization process involving the user is proposed to address the computational challenges posed by large design problem instances. The case study of the Province of Quebec is used to evaluate the performance of the proposed resolution approach.

1. Introduction

The intensifying climate crisis, driven by GreenHouse Gas (GHG) emissions generated by fossil fuels and the depletion of fossil fuel reserves, has forced countries around the world to explore alternative energy sources (Zheng et al., 2023), such as first and second-generation biofuels. Second-generation biofuels are more sustainable, not least because they are derived from non-food plant or crop residues (e.g., corn stover), unlike first-generation biofuels which are made from edible crops (Valladares-Diestra et al., 2022). In addition, second-generation biofuels are increasingly recognized as an attractive alternative because they can partially replace fossil fuels in the transportation sector and significantly reduce GHG emissions (Mofijur et al., 2016). In this respect, a regulation was adopted in December 2021 by the Government of Quebec on the integration of low-carbon fuel content into gasoline and diesel (Williams, 2022). In 2023, Quebec will require 10% low-carbon fuel content in gasoline and 3% in diesel, increasing to 15% and 10%, respectively, by 2030 (Government of Canada, 2022). In this context, creating an industrial symbiosis to produce second-generation biofuels from corn residues is a promising avenue. In addition to the environmental benefits, such as reducing the demand for fossil fuels and valorizing waste, this symbiosis offers existing companies in Quebec, including corn farmers, the possibility to enhance their profitability by creating new market opportunities.

Biofuel production from biomass faces challenges in designing the supply chain network (Maillé and Frayret, 2016; Liu et al., 2013; Bai et al., 2011). More than 44% of the total selling price of biofuels can be attributed to biomass production, logistics, and processing operations involved in converting biomass into feedstock (Roni et al., 2019). Of these expenses, logistics costs typically account for between 20% and 50% of the total feedstock costs (Djomo et al., 2023). Consequently, reducing feedstock expenses can play a crucial role in decreasing the overall costs associated with the biofuel supply chain network.

Motivated by a real-world case in Quebec, the present paper aims to enhance the environmental and economic efficiency of the province by developing a decision-support system to design a symbiotic network valorizing corn biomass and generating second-generation biofuels. First, the paper puts forth a distributed decision-making system, involving multiple actors collaborating in strategic exchanges to efficiently align waste and coproduct sources with the requirements of biofuels customers. Second, to take into account the interests of the symbiosis

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actors, a non-cooperative game theory is considered, and a Distributed Decision-Making (DDM) model is proposed. Based on a four-actor Stackelberg–Nash game, the DDM model enables the determination of the number, capacity, and location of biomass processing depots. In addition, the DDM model allows for the determination of purchase prices, biomass supply levels (corn residue supplied by farmers), as well as sales prices and production levels for the primary product (cellulosic sugar) and coproducts (hemicelluloses and lignin). The DDM model is solved using the Karush–Kuhn–Tucker (KKT) method, which generates nonlinear conditions. After linearizing these conditions, the complexity of the model increases significantly. Thus, a three-step optimization process, using clustering and involving the user, is developed to tackle and resolve the model.

The remainder of this paper is organized as follows. Section 2 provides a concise review of the literature on models for designing biofuel supply chain networks and DDM models in general. Section 3 introduces the problem statement. Section 4 presents the industrial symbiosis as a DDM system, as well as the DDM model. While the resolution approach is provided in Section 5, the numerical results are presented in Section 6. In Section 7, the main findings will be discussed. Section 8 includes conclusions and some recommendations.

2. Literature review

This section is divided into two parts. The first part focuses on models for designing biofuel supply chain networks, while the second part presents distributed decision-making models and resolution methods commonly used to support group decision-making in large and complex systems.

2.1. Models for designing Biofuel Supply Chain Networks (BSCNs)

The papers that were identified and analyzed during this part have been classified into two categories: linear or traditional BSCN and Symbiotic BSCN, an expansion of traditional BSCN.

2.1.1. Linear BSCNs

The literature presents various models for the design of linear BSCNs and for optimizing flows of raw materials and products. A comprehensive optimization strategy has been formulated by Shirazaki et al. (2024) for the creation of a microalgae biofuel system. The approach begins by refining the biorefinery architecture for microalgae biomass. Following this, it integrates a carbon capture, utilization, and storage framework. To tackle uncertainties in key input parameters, a resilient optimization model is utilized. Santibañez-Aguilar et al. (2016) introduced a linear mixed model to determine the optimal design decisions under different feedstock price scenarios, taking into account the environmental and economic impacts of the annual net profit of the biorefinery. The authors concluded that feedstock price uncertainty primarily influences the optimal network structure, with no significant impact on profitability or environmental considerations. Along this line, Roni et al. (2017) developed a multi-objective linear mixed model that integrates both environmental and social objectives. Through a real-world case study conducted in North Dakota, the model provides a HUB-and-spoke supply chain design that optimizes biomass transportation costs, the number of jobs created, and the CO_2 emissions generated by transportation activities. Recently, Afkhami and Zarrinpoor (2022) have developed a two-stage approach to design and optimize a supply chain network producing biofuel from Jatropha Curcas (a species of flowering plant) and cooking oil. The first phase uses a geographic information system (GIS) to analyze the environmental and geological characteristics of Jatropha Curcas farm locations. The second phase optimizes the BSCN using a multi-objective linear model. Roni et al. (2019) developed a Mixed Integer Linear Programming (MILP) model to evaluate the best way to use biomass and how a distributed BSCN could increase the drawing area and the supply volume compared to the centralized BSCN. The authors proposed also a dynamic approach to meet the feedstock quality specifications.

In the context of sustainable strategies and resource management within biofuel supply chains, Ghani et al. (2018) developed a decision-making tool that uses a linear model to identify biomass-producing agricultural farms (corn residues) in need of subsidies to convert their residues into bioethanol. By incorporating emission penalties, the tool can also determine the appropriate mode of transportation. A multi-objective multi-period MILP model was developed by Mahjoub et al. (2020) for the design of a second and third-generation BSCN. This model integrates anaerobic digestion and transesterification processes and considers three types of biomass sources: agricultural residues and livestock manure, microalgae, and jatropha.

2.1.2. Symbiotic BSCNs

In the literature, industrial symbiosis is an extension of the traditional supply chain that includes symbiotic suppliers and buyers, as well as resource or information-sharing firms (Turken and Geda, 2020). A symbiotic BSCN is generally based on collaborative strategies involving different industries (Martin et al., 2009; Martin, 2015). The primary goal of symbiosis is to convert by-products (i.e., products that are produced anyway as a result of the processing but are often considered as waste (Lehoux et al., 2012)) into valuable products. In the context of a BSCN, corn residues are considered by-products that can be converted into cellulosic sugar (the main product) and pig feed (a coproduct that results in producing the main product). There are few studies in the literature that focus on symbiotic relationships. Nguyen et al. (2024) presented the development and analysis of an industrial symbiosis system designed to utilize regional crop residues for the production of energy and chemicals. The research focuses on creating an integrated approach that leverages locally available agricultural by-products to enhance resource efficiency and sustainability. By evaluating the potential of crop residues as feedstocks, the study aims to optimize the generation of valuable products while reducing waste and environmental impact. Martin and Eklund (2011) exposed the benefits of an industrial symbiosis producing first and second-generation biofuels. In contrast to this study which does not conduct a quantitative analysis, Gonela and Zhang (2014) proposed Linear Programming (LP) and MILP models to determine the optimal configuration of a bioenergy-based industrial symbiosis and to optimize the network flows of a BSCN. Along this line, Li et al. (2021) proposed another model to design an industrial symbiosis that generates second and third-generation biofuels. Their model considers the multiple interactions of the BSCN actors, which allows them to reduce the annual manufacturing cost (Capital and biofuel production costs) by more than 10% in all IS scenarios and to reduce GHG emissions by 36%. None of the above-mentioned studies provided a multi-period model to address the joint design and pricing problem for symbiotic BSCN, as proposed by this paper.

2.2. Models and resolution methods for Distributed Decision-Making (DDM)

This section delves into the various approaches and techniques used to understand and address the complexities of decision-making in distributed environments.

2.2.1. Models for Distributed Decision-Making

Distributed models are predominant in handling decision-making in complex systems such as BSCNs. They have not only to deal with subsystems' problems but are mainly concerned with the coordination task (Schneeweiss, 2012). In the literature related to supply chain networks design and planning, several distributed models are used to optimize cooperative DDM systems. Gjerdrum et al. (2001) presented a mathematical programming model using Nash-type game theory for fair profit distribution in multi-enterprise supply chains, formulating it as a mixed-integer nonlinear programming problem. The approach

is refined into a mixed-integer linear programming model and validated through case studies. In a subsequent study, Gjerdrum et al. (2002) introduced a mathematical programming model for fair profit distribution in multi-enterprise supply chains using the Nash bargaining solution, formulated as a mixed-integer nonlinear programming (MINLP) problem. It employs a branch-and-bound algorithm with exact and approximate linearizations to solve this model, optimizing inter-firm transfer prices, production levels, inventory, and product flows, with its applicability demonstrated through industrial case studies. Also, Taghipour and Frayret (2012) proposed a decentralized coordination mechanism for supply chains, based on negotiation-like mutual adjustments of planning decisions, to address the challenges of information sharing in decentralized systems. The approach, which involves interaction between two enterprises to enhance both individual and collective performance, achieves near-optimal results and equitable revenue sharing compared to centralized systems. Zhang et al. (2013) presented a mathematical programming model for fair cost distribution in microgrids, using the Nash bargaining solution approach to optimize multi-partner cost levels within specified cost bounds. The problem, initially formulated as a mixed-integer nonlinear programming model, is transformed into a mixed-integer linear programming model through separable programming, and applied to a case study involving five microgrid participants. In addition, Fernandes et al. (2013) developed a deterministic mixed-integer linear program (MILP) for optimizing the strategic design and planning of a multi-entity, multi-echelon petroleum supply chain network. The MILP determines optimal depot locations, capacities, transportation modes, routes, and network configurations to maximize long-term profits across the supply, refining, distribution, and retail stages, and is tested using a real-case network in Portugal. For the non-cooperative DDM systems, Ryu et al. (2004) modeled supply chain optimization as a bilevel programming, using parametric programming to solve plant and distribution network problems optimally. Also, Zamarripa et al. (2012) extended a Mixed Integer Linear Programming (MILP) model for supply chain planning by integrating Game Theory, testing it with a case study involving two supply chains and two optimization criteria for competitive scenarios. In addition, Zamarripa et al. (2013) introduced third parties to supply chain planning, modeled the interaction with the supply chain, employed multi-objective optimization to handle competition trade-offs, and used game theory for reactive decision-making.

Since BSCNs are typically decentralized and involve multiple actors, a DDM model enables the consideration of the objectives of each actor and the common Leader-Follower hierarchy structure. For example, to design a second-generation BSCN, Yue and You (2014) developed a single-period DDM model based on the Stackelberg game. This model specifically addresses the pricing problem by establishing equilibrium through fictitious markets. The authors have also developed a global solution method that considerably reduces computational time compared to commonly used commercial solvers such as BARON and SCIP. The current paper, unlike (Yue and You, 2014), considers the symbiotic aspect and thus proposes a game-theoretic model incorporating more optimization levels. Similarly, Jonkman et al. (2019) propose a game-theoretic model considering two key actors (farmers and biomass processing facilities) and addressing the biomass pricing problem. The current paper considers a more complex distributed problem incorporating four actors and deals with coproduct pricing, in addition to biomass pricing.

2.2.2. Resolution methods for Distributed Decision-Making

The resolution of Leader-Follower DDM models is typically achieved using two different types of methods: classical methods and evolutionary methods (Sinha et al., 2017).

Classical methods

One widely used classical method relies on Karush–Kuhn–Tucker (KKT) optimality conditions. This method is applicable for bi-level models with a convex low-level problem. The idea is to replace the low-level problem with the appropriate optimality conditions at the high level. Following this transformation, a new mathematical model is obtained with equilibrium constraints, which can be solved using classical resolution approaches such as Branch and Bound or classical heuristics and metaheuristics methods. For example, Bialas and Karwan (1984) explored two-level linear programming problems within decentralized planning, focusing on how hierarchical control structures allow for influencing policies at different levels. The authors presented geometric characterizations and algorithms to show the tractability of these problems and encourages further research. Also, Chen and Florian (1992) analyzed the structure of linear bilevel program solutions by examining the dual polyhedron of the lower level problem, demonstrating that optimal solutions occur at the vertices of a connected dual inducible region and outlining methods for solving these problems. In addition, Tuy et al. (1993) reformulated linear two-level programming problems, often related to Stackelberg leader-follower games, as global optimization problems and developed a new solution method leveraging recent global optimization techniques, illustrated with a small example. Besides, Zhang et al. (2023) proposed a leader-follower bi-level model for microgrid energy management, using Stackelberg game theory and stochastic MPEC, validated by numerical results. Last but not least, Han et al. (2023) proposed a privacy-preserving bilevel optimization for microgrids using Stackelberg games and Benders decomposition, validated by numerical tests. A second classical method is similar to the previous method but introduces a penalty function. The penalty can be associated with both levels of the bi-level model before applying the KKT reformulation (Ishizuka and Aiyoshi, 1992), or it can be added only to the complementarity condition generated by the KKT approach (Lv et al., 2007).

Evolutionary methods

Evolutionary resolution approaches encompass nested methods and methods that reduce the problem to a single-level problem (Sinha et al., 2017). For nested methods, specific algorithms are required to solve each level and high-level solutions are considered to determine the solutions of the low-level problem (Sinha et al., 2017). For example, Mathieu et al. (1994) used a genetic algorithm to solve the high-level problem, while they applied a classical method of solving linear programs for the low-level problem. Similarly, Zhu et al. (2006) used a method based on differential evolution to solve the high-level problem and the interior point method to solve the low-level problem. In contrast to nested methods, reducing the problem to a single-level problem requires the low-level of the problem to be convex and to exhibit certain regularities. Regularities imply that the objective function and constraints are defined consistently, and an example of regularity is the smoothness of the objective function. This approach based on single-level reduction has been generalized to apply to bi-level problems regardless of context (Sinha et al., 2017). For example, Hejazi et al. (2002) solved the equilibrium-constrained mathematical program, obtained from the KKT reformulation, using a genetic algorithm with chromosomes representing the vertices of the polyhedron solution.

2.3. Research gaps and contribution of the paper

Although this literature offers various solutions for designing BSCNs, none of them addresses both the need to incentivize biomass providers to sell their by-products (biomass pricing optimization) and the need to maximize the profit of processing depots by valorizing coproducts (coproduct pricing optimization). Building on Yue and You (2014), a new multi-period game-theoretic model is proposed to optimize the symbiotic BSCN design and product pricing within a market equilibrium. This paper is the first to consider four actors (corn farms, processing depots managed by a HUB, biorefineries, and pig farms) when making decisions on the biomass-to-bioenergy supply chain. Furthermore, this paper deals with a multi-product biomass-to-bioenergy supply chain (cellulosic sugar for second-generation biofuel and a coproduct as animal feed), whereas most studies focus on a single product. Finally, this paper proposes a novel resolution approach for distributed models based on data clustering and interactive reoptimization.

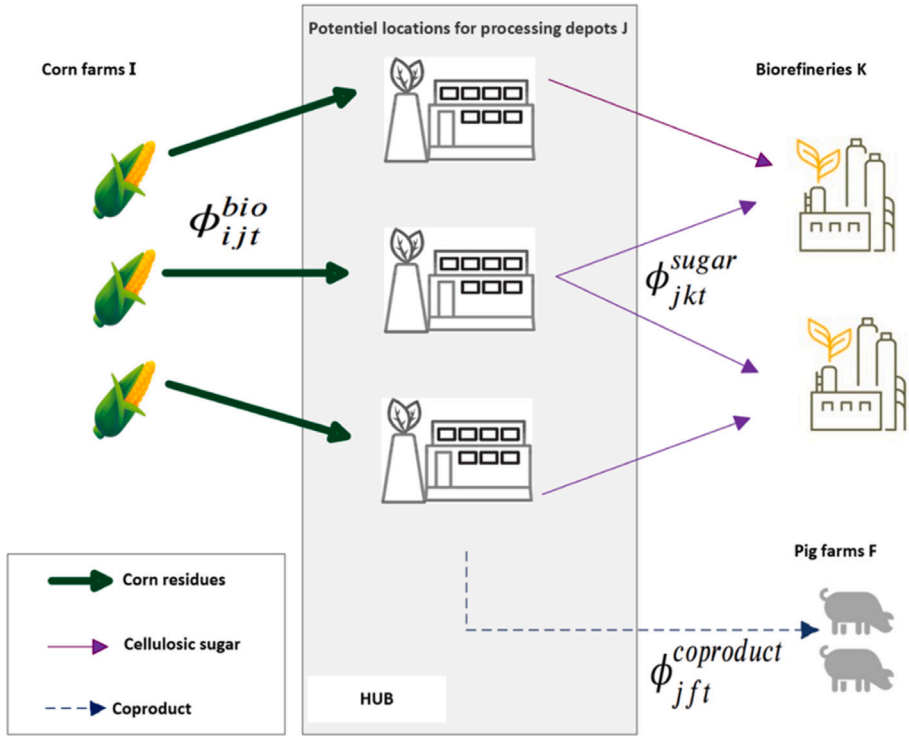


Fig. 1. The industrial symbiosis proposed to produce second-generation biofuels from corn residues.

3. Problem statement

As briefly introduced above, this paper addresses the problem of designing an industrial symbiosis to produce second-generation biofuels from corn residues. In this context, an actor is only interested in participating in the symbiosis if his participation increases his profit. The idea of symbiosis can be considered less attractive if the revenues do not exceed the costs (e.g., biomass production, logistics, and processing operations). Therefore, a decision-support system is needed to guarantee an optimal profit for the different actors of the symbiosis. This system can be particularly useful for Quebec, the second largest corn-producing province in Canada (Hamel and Dorff, 2014), where the idea of a BSCN can be interesting to improve the environmental and economic efficiency of the province. The design problem can be described as follows. Given **I** existing corn farms, a decision needs to be made on where to locate processing depots among **J** potential locations. Processing depots, supplied by corn farms, offer two products: cellulosic sugar to **K** biorefineries and pig feed to **F** pig farmers. For the sake of simplicity, the terms "sugar" and "coproduct" will be used in the following sections and refer to "cellulosic sugar" and "pig feed", respectively.

The presence of processing depots in conjunction with biorefineries offers several advantages. Corn residues can be valorized and transformed into sugar and coproduct. Processing depots can also offer the lowest price to the local customers since transportation costs are reduced. However, depots address challenges such as flowability, transportability, stability, and storage (Geismar et al., 2022). Given the multi-level structure of this BSCN, a central HUB is introduced to make strategic and tactical decisions aimed at maximizing the overall profit of all processing depots. The structure of the BSCN proposed is illustrated by Fig. 1. For each period (e.g., a year), the HUB needs to determine (a) the number and the locations of the depots (one decision-maker), (b) the production capacity and the supply of each depot, (c) the corn residues prices offered to corn farmers, and (d) the selling prices of the sugar and the coproduct offered to biorefineries and pig farms, respectively. Therefore, the HUB can be considered as the leader of the BSCN, while both the suppliers (corn farmers) and the customers (biorefineries and pig farmers) can be considered as followers. A non-cooperative context is assumed, where independent decisions are made by the followers in response to the leader's actions. This situation can be formulated as a Stackelberg game.

For the followers (corn farmers, biorefineries, and pig farmers), a static game (i.e., a strategic situation in which the actors simultaneously decide on their strategy (Mahmoodi, 2020)) can be observed. In this study, this static game is chosen for analysis under Nash equilibrium (i.e., a situation in which none of the actors can modify their payoff by deviating from their decision while the others' strategies are fixed (Mahmoodi, 2020)). Thus, it is assumed that followers make their decisions simultaneously and compete over quantities and prices in a common market. In this context, the optimal final decisions of the BSCN design problem are a Stackelberg–Nash equilibrium.

In response to the leader's decisions, each follower maximizes his profit simultaneously with the other followers. For each period t, each corn farmer i decides how much biomass to sell to each processing depot, each pig farm f decides how much to purchase from each processing depot, and each biorefinery k decides how much sugar to purchase from each depot.

For the leader (i.e., the HUB), it is essential to carefully determine the prices offered to farmers and customers. If the biomass price is set too low, corn farms may refuse to sell to processing depots (not a profitable situation). Conversely, if the price is set too high, the depot would increase raw material costs. The same challenge is faced by customers: if the price offered by depots is set too high, biorefineries and pig farms may be hesitant to buy. Conversely, if the price is set too low, the depot would miss out on potential revenue. Furthermore, if the HUB finds it unprofitable to invest in the BSCN, no processing depots would be opened.

4. Mathematical model

This paper proposes a Distributed Decision-Making (DDM) model that aims to support decision-making with the 4 types of actors of our

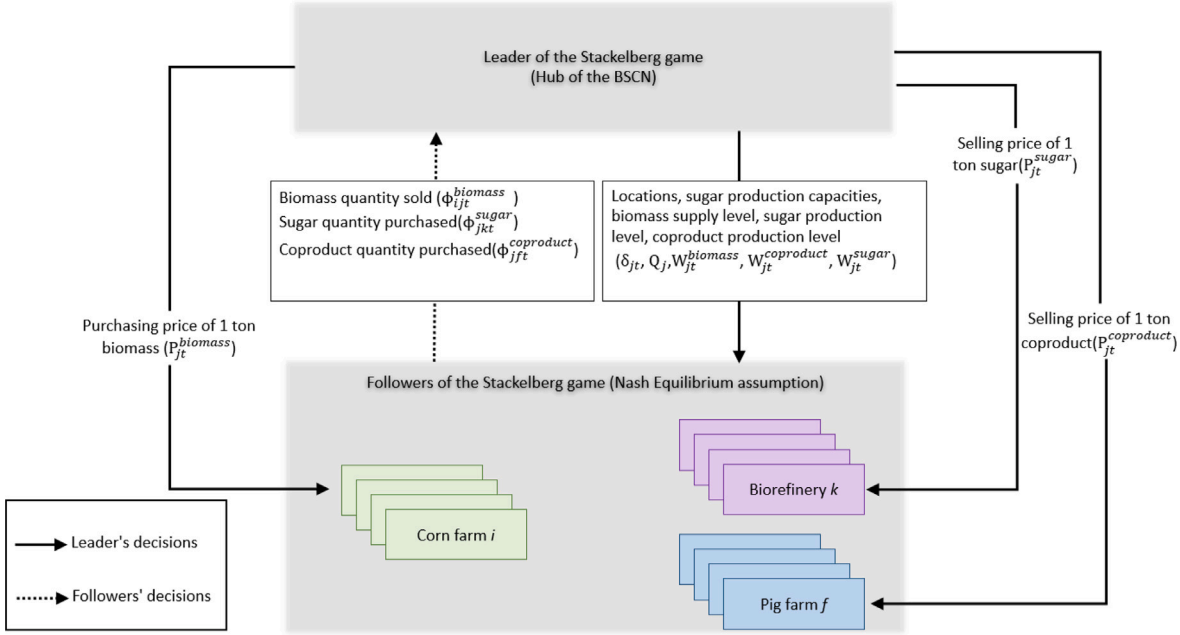


Fig. 2. Distributed decision-making through the symbiotic Biofuel Supply Chain Network (BSCN).

Table 1
Indexes used in modeling.

Indexes	
i	Corn farm (i = 1..I)
j	Potential location j for processing depots (j = 1..**J**)
k	Biorefinery (k = 1..**K**)
f	Pig farm (f = 1..**F**)
t	Period (t = 1..**T**)

BSCN (Fig. 2). In short, the hierarchical leader (HUB) of this DDM system first optimizes the locations, sugar production capacities, and supply and production levels of the depots. From this optimization process, it also derives the selling prices of the sugar for the biorefinery and the coproduct for the pig farms, as well as the prices offered to the corn farms for the purchase of their by-products (i.e., corn residues). Once the leader's decisions are sent to their respective actors, the followers independently optimize their production process to decide how much corn residue to sell at the sales price proposed by the HUB, and how much sugar and coproduct to procure at the purchase prices offered by the HUB. The followers' decisions are sent back to the leader. To carry out this process, several interrelated optimization models must be used. The next section describes each of these models.

4.1. Distributed Decision-Making (DDM) model

This section describes four optimization models, starting with the leader (the HUB), then the corn farmers, the biorefineries, and the pig farmers. To standardize all models, the following notations and indexes are described hereafter through Tables 1 to 5.

4.1.1. HUB (leader) problem

A first model is required by the HUB to make decisions related to processing depots' locations, capacity planning, and pricing problems. Table 2 presents the notation used to formulate this model. The main objective of the HUB is to maximize the total profit from all the processing depots over the entire planning horizon as given by the objective function (FO1). The first term of (FO1) corresponds to the revenue generated from selling sugar to biorefineries, which is calculated as the product of the sugar price (P_{jt}^{sugar}) and the total sales amount (Φ_{jkt}^{sugar}). The second term represents the revenue generated from selling the coproduct to pig farms. The third term represents the sale of surplus coproducts to the external market once the demand of the pig farms has been met. The fourth term corresponds to the sale of surplus sugar on the external market, once the demand of the biorefineries has been met. The HUB's costs mainly include the purchase cost of biomass from corn farmers, investments in depot construction, operating costs associated with running the depots, as well as the purchase of additional biomass on the external market if the farmers are unable to supply the quantity of biomass required to fill the quantity required by the depots ($W_{jt}^{biomass}$).

Eqs. (1) and (2) express the sale of surplus of sugar and coproduct by the depots. Eq. (3) determines the cost of the quantity of biomass that needs to be purchased by the depots from the external market, which offers a higher price than farmers. Eqs. (4)–(11) describe the various production and depot opening constraints. More specifically, Eq. (4) ensures that the amount of sugar produced in a processing depot cannot exceed its capacity. Eqs. (5)–(7) stipulate that if the processing depot is not open, the corresponding sales of sugar and coproduct ($\sum_{k\in K}\phi_{jkt}^{sugar}$ and $\sum_{f\in F}\phi_{jft}^{coproduct}$), as well as the biomass supply, ($W_{jt}^{biomass}$) should be zero. In other words, sales and purchases can only be carried out when the processing depot is open. Eq. (8) reveals that sugar production capacity is limited and cannot exceed a certain maximum capacity value (q_{max}). Eqs. (9) and (10) ensure the conversion from biomass to sugar and to coproduct at the processing depot. In other words, the amount of sugar and coproduct generated depends directly on biomass availability and is governed by the conversion factors α and μ. Finally, Eq. (11) ensures that all variables used are positive values, except those determining the locations of the depots (δ_{jt}) which are binary.

$$\max \Pi^J(P_{jt}^{sugar}, P_{jt}^{coproduct}, P_{jt}^{biomass}, \delta_{jt}, W_{jt}^{biomass}, W_{jt}^{sugar}, W_{jt}^{coproduct}, Q_j)$$
$$= \sum_{t\in T}\sum_{k\in K}\sum_{j\in J} P_{jt}^{sugar}\phi_{jkt}^{sugar}$$
$$+ \sum_{t\in T}\sum_{f\in F}\sum_{j\in J} P_{jt}^{coproduct}\phi_{jft}^{coproduct} + S^{coproduct} + S^{sugar}$$
$$- \sum_{t\in T}\sum_{i\in I}\sum_{j\in J} P_{jt}^{biomass}\phi_{ijt}^{biomass} - \sum_{j\in J} c^{fix}Q_j$$
$$- \sum_{t\in T}\sum_{j\in J} c^{coproduct}W_{jt}^{coproduct} - \sum_{t\in T}\sum_{j\in J} c^{sugar}W_{jt}^{sugar} - S^{biomass} \quad (FO1)$$

Table 2
The HUB parameters and decision variables.

Parameters	
α	Conversion factor of corn residue to sugar
μ	Conversion factor of corn residue into coproduct
$c^{coproduct}$	Cost of obtaining 1 ton of coproduct from the biomass
c^{sugar}	Cost of obtaining 1 ton of sugar from the biomass
c^{fix}	Fixed cost for constructing a depot with a 1-ton capacity
$mc_t^{coproduct}$	Cost of purchasing 1 ton of coproduct for a pig farm at period t on the external market
mc_t^{sugar}	Cost of purchasing 1-ton sugar from the external market for a biorefinery at period$t$
$m_t^{biomass}$	External Market price of 1 ton biomass at period t
$m_t^{coproduct}$	External Market price of 1 ton coproduct at period t
m_t^{sugar}	External Market price of 1-ton coproduct sugar at period t
q_{max}	Maximum sugar quantity that can be produced by a depot
Big M	A very large number
Decision variables	
$W_{jt}^{biomass}$	Biomass supply level set by a depot at location j at period t
$W_{jt}^{coproduct}$	Coproduct production level set by a depot at location j at period t
W_{jt}^{sugar}	Sugar production level set by a depot at location j at period t
Q_j	Sugar production capacity of a depot at location j
$P_{jt}^{coproduct}$	Selling price of 1-ton coproduct by a depot at location j at period t
P_{jt}^{sugar}	Selling price of 1-ton sugar by a depot at location j at period t
$P_{jt}^{biomass}$	Purchasing price of 1-ton biomass set by a depot at location j at period t
δ_{jt}	Binary variable equal to 1 if a depot at location j is open at period t; 0 otherwise
$S^{coproduct}$	Total profit from selling surplus of coproduct to the external market
S^{sugar}	Total profit from selling surplus of sugar to the external market
$S^{biomass}$	Total purchasing cost of additional biomass quantity required to fill the demand
Π^J	Total profit of all processing depots

$$S^{coproduct} = \sum_{t\in T}\sum_{j\in J} m_t^{coproduct}(W_{jt}^{coproduct} - \sum_{f\in F}\phi_{jft}^{coproduct}) \tag{1}$$

$$S^{sugar} = \sum_{t\in T}\sum_{j\in J} m_t^{sugar}(W_{jt}^{sugar} - \sum_{k\in K}\phi_{jkt}^{sugar}) \tag{2}$$

$$S^{biomass} = \sum_{t\in T} m_t^{biomass}(\sum_{j\in J} W_{jt}^{biomass} - \sum_{i\in I}\sum_{j\in J}\phi_{ijt}^{biomass}) \tag{3}$$

$$W_{jt}^{sugar} \le Q_j, \forall j \in J, \forall t \in T \tag{4}$$

$$\sum_{f\in F}\phi_{jft}^{coproduct} \le bigM * \delta_{jt}, \forall j \in J, \forall t \in T \tag{5}$$

$$\sum_{k\in K}\phi_{jkt}^{sugar} \le bigM * \delta_{jt}, \forall j \in J, \forall t \in T \tag{6}$$

$$W_{jt}^{biomass} \le bigM * \delta_{jt}, \forall j \in J, \forall t \in T \tag{7}$$

$$Q_j \le q_{max} * \delta_{jt}, \forall j \in J, \forall t \in T \tag{8}$$

$$W_{jt}^{sugar} = \alpha * W_{jt}^{biomass}, \forall j \in J, \forall t \in T \tag{9}$$

$$W_{jt}^{coproduct} = \mu * W_{jt}^{biomass}, \forall j \in J, \forall t \in T \tag{10}$$

$$W_{jt}^{sugar}, W_{jt}^{coproduct}, W_{jt}^{biomass}, P_{jt}^{biomass}, P_{jt}^{sugar}, P_{jt}^{coproduct}, Q_j \ge 0, \delta_{jt} \in \{0,1\} \tag{11}$$

4.1.2. Corn farm problem

Table 3 presents the notation used to formulate the problem of a corn farm i. Each corn farm i aims to maximize its profits by estimating the profits of the other farmers since each biomass supplier in the supply chain is independent. Therefore, the decisions of other farms are treated as constants from the farm i's perspective under the assumption of Nash equilibrium. This objective is formulated in the objective function (FO2), where a farmer's profit is determined by the difference between the revenues of the biomass sold and the transportation costs associated with shipping the biomass to the processing depots. The constraints of the corn farms problem are expressed in Eqs. (12)–(14). Eq. (12) aims to limit the quantity of biomass sold by a farm i at period t so that it does not exceed the quantity of biomass available at that farm. In addition, Eq. (13) guarantees that the total quantity of biomass sold by all farmers to a processing depot at period t does not exceed the depot's biomass supply level ($W_{jt}^{biomass}$) set by the HUB. Eq. (14) guarantees that the quantity of biomass sold and transported is a positive value.

$$\max \Pi^i(\phi_{ijt}^{biomass}) = \sum_{t\in T}\sum_{j\in J}(P_{jt}^{biomass} - tc^{fix,biomass} - tc^{var,biomass}d_{ij})\phi_{ijt}^{biomass} \quad (FO2)$$

$$\sum_{j\in J}\phi_{ijt}^{biomass} \le \eta^I * r_{it}, \forall t \in T \tag{12}$$

$$\sum_{i'\in I}\phi_{i'jt}^{biomass} \le W_{jt}^{biomass}, \forall j \in J, \forall t \in T \tag{13}$$

$$\phi_{ijt}^{biomass} \ge 0, \forall j \in J, \forall t \in T \tag{14}$$

4.1.3. Biorefinery problem

Table 4 presents the notation used to formulate the problem of a biorefinery k. After anticipating the decisions of the other biorefineries, a biorefinery k seeks to maximize its profits by reducing its purchases from the external market, as described in the objective function (FO3). Eq. (15) ensures that the quantity of sugar sold by all depots in a period t does not exceed the biorefinery demand. Eq. (16) guarantees that the quantity of sugar purchased by all the biorefineries from a processing depot at a period t does not exceed the production level of the processing depot at location j (W_{jt}^{sugar}). Finally, Eq. (17) ensures that the variable representing the quantity of sugar sold and transported from a depot at location j to biorefinery k is positive.

$$\max \Pi^k(\phi_{jkt}^{sugar}) = \sum_{t\in T}\sum_{j\in J}(mc_t^{sugar} - (P_{jt}^{sugar} + tc^{fix,sugar} + tc^{var,sugar}d_{jk}))\phi_{jkt}^{sugar} \quad (FO3)$$

$$\sum_{j\in J}\phi_{jkt}^{sugar} \le \varphi_{kt}^{sugar}, \forall t \in T \tag{15}$$

$$\sum_{k'\in K}\phi_{jk't}^{sugar} \le W_{jt}^{sugar}, \forall j \in J, \forall t \in T \tag{16}$$

$$\phi_{jkt}^{sugar} \ge 0, \forall j \in J, \forall t \in T \tag{17}$$

Table 3
Corn farmers parameters and decision variables.

Parameters	
$tc^{fix,biomass}$	Fixed cost of transporting 1 ton biomass
$tc^{var,biomass}$	Variable cost of transporting 1 ton biomass per kilometer
d_{ij}	Distance between corn farm i and a depot at location j
r_{it}	Quantity of biomass available at corn farm i at period t
η^I	Participation ratio of the I corn farms
Decision variables	
$\phi^{biomass}_{ijt}$	Biomass quantity sold by from corn farm i to a depot at location j at period t
Π^i	Total profit of the corn farm i

Table 4
Biorefineries parameters and decision variables.

Parameters	
$tc^{fix,sugar}$	Fixed cost of transporting 1 ton sugar
$tc^{var,sugar}$	Variable cost of transporting 1 ton sugar per kilometer
d_{jk}	Distance between a depot at location j and biorefinery k
φ^{sugar}_{kt}	Quantity of sugar required by biorefinery k at period t
Decision variables	
ϕ^{sugar}_{jkt}	Sugar quantity purchased from a depot at location j to biorefinery k at period t
Π^k	Total profit of biorefinery k

Table 5
Pig farms parameters and decision variables.

Parameters	
$tc^{fix,coproduct}$	Fixed cost of transporting 1 ton coproduct
$tc^{var,coproduct}$	Variable cost of transporting 1 ton coproduct per kilometer
d_{jf}	Distance between a depot at location j and pig farm f
$\varphi^{coproduct}_{ft}$	Quantity of coproduct required by pig farm f at period t
Decision variables	
$\phi^{coproduct}_{jft}$	Coproduct quantity purchased from a depot at location j to pig farm f at period t
Π^f	Total profit of pig farm f

4.1.4. Pig farm problem

Table 5 presents the notation used to formulate the problem of a pig farm f. After anticipating the decisions of the other farms, a pig farm aims to maximize its profits by minimizing its purchases on the external market, as given by the objective function (FO4). The constraints related to the pig farm problem are similar to those of the biorefinery problem. Eq. (18) ensures that the quantity of coproduct sold by all processing depots in a period t must not exceed the pig farm's demand ($\varphi^{coproduct}_{ft}$). Eq. (19) states that the quantity of coproduct purchased by all the pig farms from a processing depot at a period t does not exceed the production level of the processing depot at location j. Finally, Eq. (20) ensures that the variable representing the quantity of coproduct sold and transported from a depot at location j to pig farm f is positive.

$$\max \Pi^f(\phi^{coproduct}_{jft}) = \sum_{t\in T}\sum_{j\in J}(mc^{coproduct}_t - (P^{coproduct}_{jt} + tc^{fix,coproduct} + tc^{var,coproduct}d_{jf})) \times \phi^{coproduct}_{jft} (FO4)$$

$$\sum_{j\in J}\phi^{coproduct}_{jft} \le \varphi^{coproduct}_{ft}, \forall t \in T \tag{18}$$

$$\sum_{f'\in F}\phi^{coproduct}_{jf't} \le W^{coproduct}_{jt}, \forall j \in J, \forall t \in T \tag{19}$$

$$\phi^{coproduct}_{jft} \ge 0, \forall j \in J, \forall t \in T \tag{20}$$

4.2. Reformulation of the DDM model

The DDM model formulated above addresses a multilevel problem with several optimization subproblems that cannot be directly handled by off-the-shelf mathematical programming solvers due to their limited computational performance on large-scale applications. In this section, a proposal is made to reformulate this multilevel model, which comprises mixed variables (continuous and integer), into a single-level model. This can be accomplished by using the Karush–Kuhn–Tucker (KKT) condition-based approach instead of the nesting-based approach. In fact, according to Sinha et al. (2017), nesting approaches are less suitable for large-scale problems such as ours. First, the KKT conditions associated with the followers' problems, formulated in Section 4.1, have been incorporated as linear programs. These conditions were then embedded into the leader's constraints to obtain a single-level model.

4.2.1. KKT conditions applied to followers' problems

Given a general problem:

$$Min_{x\in X}\, k(x, y)$$

s.t

$$m(x, y) \le 0$$

The KKT conditions, also known as optimality conditions for an optimization problem, consist of four sets of constraints, namely stationarity (21), primal feasibility (22), dual feasibility (23), and complementary slackness (24), where $L(x, y, v) = k(x, y) + v^T m(x, y)$ and v is the Lagrange multiplier associated to the optimization problem.

$$\nabla_y L(x, y, v) = 0 \tag{21}$$

$$m(x, y) \le 0 \tag{22}$$

$$v \geq 0 \tag{23}$$

$$v^T m(x, y) = 0 \tag{24}$$

By applying the principle described above, the corn farm problem is replaced by constraints (12)–(14) and (25)–(31), where $\beta^1_{it}, \beta^2_{jt}, \beta^3_{ijt}$ are the Lagrange multipliers associated respectively with initial constraints (12)–(14).

$$\sum_{j\in J} \phi^{biomass}_{ijt} - \eta^I r_{it} \leq 0, \forall i \in I, \forall t \in T \tag{12}$$

$$\beta^1_{it}(\sum_{j\in J} \phi^{biomass}_{ijt} - \eta^I r_{it}) = 0, \forall i \in I, \forall t \in T \tag{25}$$

$$\beta^1_{it} \geq 0, \forall i \in I, \forall t \in T \tag{26}$$

$$\sum_{i\in I} \phi^{biomass}_{ijt} - W^{biomass}_{jt} \leq 0, \forall j \in J, \forall t \in T \tag{13}$$

$$\beta^2_{jt}(\sum_{i\in I} \phi^{biomass}_{ijt} - W^{biomass}_{jt}) = 0, \forall j \in J, \forall t \in T \tag{27}$$

$$\beta^2_{jt} \geq 0, \forall j \in J, \forall t \in T \tag{28}$$

$$-\phi^{biomass}_{ijt} \leq 0, \forall i \in I, \forall j \in J, \forall t \in T \tag{14}$$

$$-\beta^3_{ijt}\phi^{biomass}_{ijt} = 0, \forall i \in I, \forall j \in J, \forall t \in T \tag{29}$$

$$\beta^3_{ijt} \geq 0, \forall i \in I, \forall j \in J, \forall t \in T \tag{30}$$

The stationarity condition (31) related to this optimization problem is added.

$$-P^{biomass}_{jt} + tc^{fix,biomass} + tc^{var,biomass} d_{ij} + \beta^1_{it} + \beta^2_{jt} - \beta^3_{ijt} = 0, \forall i \in I, \forall j \in J, \forall t \in T \tag{31}$$

Similarly, the biorefinery problem is replaced by constraints (15)–(17) and (32)–(38), where γ^1_{kt}, γ^2_{jt}, γ^3_{jkt} are the Lagrange multipliers associated respectively with initial constraints (15)–(17).

$$\sum_{j\in J} \phi^{sugar}_{jkt} - \varphi^{sugar}_{kt} \leq 0, \forall k \in K, \forall t \in T \tag{15}$$

$$\gamma^1_{kt}(\sum_{j\in J} \phi^{sugar}_{jkt} - \varphi^{sucre}_{kt}) = 0, \forall k \in K, \forall t \in T \tag{32}$$

$$\gamma^1_{kt} \geq 0, \forall k \in K, \forall t \in T \tag{33}$$

$$\sum_{k\in K} \phi^{sugar}_{jkt} - W^{sugar}_{jt} \leq 0, \forall j \in J, \forall t \in T \tag{16}$$

$$\gamma^2_{jt}(\sum_{k\in K} \phi^{sugar}_{jkt} - W^{sugar}_{jt}) = 0, \forall j \in J, \forall t \in T \tag{34}$$

$$\gamma^2_{jt} \geq 0, \forall j \in J, \forall t \in T \tag{35}$$

$$-\phi^{sugar}_{jkt} \leq 0, \forall j \in J, \forall k \in K, \forall t \in T \tag{17}$$

$$-\gamma^3_{jkt}\phi^{sugar}_{jkt} = 0, \forall j \in J, \forall k \in K, \forall t \in T \tag{36}$$

$$\gamma^3_{jkt} \geq 0, \forall j \in J, \forall k \in K, \forall t \in T \tag{37}$$

The stationarity condition (38) related to this optimization problem is added.

$$-mc^{sugar}_t + P^{sugar}_{jt} + tc^{fix,sugar} + tc^{var,sugar} d_{jk} + \gamma^1_{kt} + \gamma^2_{jt} - \gamma^3_{jkt} = 0, \forall j \in J, \forall k \in K, \forall t \in T \tag{38}$$

Finally, the pig farm problem is replaced by constraints (18)–(20) and (39)–(45), where λ^1_{ft}, λ^2_{jt}, λ^3_{jft} are the Lagrange multipliers associated respectively with initial constraints (18)–(20).

$$\sum_{j\in J} \phi^{coproduct}_{jft} - \varphi^{coproduct}_{ft} \leq 0, \forall f \in F, \forall t \in T \tag{18}$$

$$\lambda^1_{ft}(\sum_{j\in J} \phi^{coproduct}_{jft} - \varphi^{coproduct}_{ft}) = 0, \forall f \in F, \forall t \in T \tag{39}$$

$$\lambda^1_{ft} \geq 0, \forall f \in F, \forall t \in T \tag{40}$$

$$\sum_{f\in F} \phi^{coproduct}_{jft} - W^{coproduct}_{jt} \leq 0, \forall j \in J, \forall t \in T \tag{19}$$

$$\lambda^2_{jt}(\sum_{f\in F} \phi^{coproduct}_{jft} - W^{coproduct}_{jt}) = 0, \forall j \in J, \forall t \in T \tag{41}$$

$$\lambda^2_{jt} \geq 0, \forall j \in J, \forall t \in T \tag{42}$$

$$-\phi^{coproduct}_{jft} \leq 0, \forall j \in J, \forall f \in F, \forall t \in T \tag{20}$$

$$-\lambda^3_{jft}\phi^{coproduct}_{jft} = 0, \forall j \in J, \forall f \in F, \forall t \in T \tag{43}$$

$$\lambda^3_{jft} \geq 0, \forall j \in J, \forall f \in F, \forall t \in T \tag{44}$$

The stationarity condition related to this optimization problem is as follows:

$$-mc^{coproduct}_t + P^{coproduct}_{jt} + tc^{fix,coproduct} + tc^{var,coproduct} d_{jf} + \lambda^1_{ft} + \lambda^2_{jt} - \lambda^3_{jft} = 0, \forall j \in J, \forall f \in F, \forall t \in T \tag{45}$$

4.2.2. Linearization of complementary slackness constraints

To linearize the KKT complementary slackness constraints previously introduced, the following binary variables are added $Z^1_{it}, Z^2_{jt}, Z^3_{ijt}, B^1_{kt}, B^2_{jt}, B^3_{jkt}, Y^1_{ft}, Y^2_{jt} and Y^3_{jft}$, associated respectively with the constraints (25), (27), (29), (32), (34), (36), (39), (41) and (43). Each binary variable takes 1 if the constraint is active, and 0 if the Lagrange multiplier is zero. Considering a huge number BM (for Big M), complementary slackness constraints are replaced as presented in Table 6.

4.2.3. Single-Level Model(SLM)

After establishing the KKT conditions for the followers' problems and linearizing the complementary slackness constraints, a Single-Level Model (SLM) formulated as a Mixed Integer Non-Linear Program (MINLP) is obtained. The SLM addresses the original multilevel problem and is composed of the objective function of the leader's problem (FO1) subject to the following constraints: (4)–(20), (26), (28), (30)–(31), (33), (35), (37)–(38), (40), (42) and ((44)–63).

5. Resolution approach

Most global optimizers for MINLPs face challenges in terms of computational performance with large-scale applications. This was the case for the SLM proposed in this study. In a previous work (Bouazizi et al., 2023), the SLM has been implemented using GAMS 42.2.0 with the BARON solver. Although a small data instance (6 corn farms, 5 potential depot locations, 1 biorefinery, and 4 pig farms) representing about 2% of the full dataset (247 corn farms, 395 potential locations for depots, and 286 pig farms) was considered, the optimizer failed to obtain an optimal solution within an 8-hour resolution time. To resolve the model using the entire dataset, this paper proposes a novel resolution approach that involves the user of the DDM system in a three-step optimization process, as illustrated by Fig. 3. First, a **clustering module** identifies clusters for corn farms, depots' potential locations, biorefineries, and pig farms according to their geographic

Table 6
Complementarity slackness constraints and corresponding linearized constraints.

Constraints	Linearized constraints	
(25)	$\beta^1_{it} \leq BM \times Z^1_{it}, \forall i \in I, \forall t \in T$	(46)
	$-(\sum_{j\in J} \phi^{biomass}_{ijt} - \eta^I r_{it}) \leq BM \times (1 - Z^1_{it}), \forall i \in I, \forall t \in T$	(47)
(27)	$\beta^2_{jt} \leq BM \times Z^2_{jt}, \forall j \in J, \forall t \in T$	(48)
	$-(\sum_{i\in I} \phi^{biomass}_{ijt} - W^{biomass}_{jt}) \leq BM \times (1 - Z^2_{jt}), \forall j \in J, \forall t \in T$	(49)
(29)	$\beta^3_{ijt} \leq BM \times Z^3_{ijt}, \forall i \in I, \forall j \in J, \forall t \in T$	(50)
	$\phi^{biomass}_{ijt} \leq BM \times (1 - Z^3_{ijt}), \forall i \in I, \forall j \in J, \forall t \in T$	(51)
(32)	$\gamma^1_{kt} \leq BM \times B^1_{kt}, \forall k \in K, \forall t \in T$	(52)
	$-(\sum_{j\in J} \phi^{sugar}_{jkt} - \varphi^{sugar}_{kt}) \leq BM \times (1 - B^1_{kt}), \forall k \in K, \forall t \in T$	(53)
(34)	$\gamma^2_{jt} \leq BM \times B^2_{jt}, \forall t \in T, \forall j \in J$	(54)
	$-(\sum_{k\in K} \phi^{sugar}_{jkt} - W^{sugar}_{jt}) \leq BM \times (1 - B^2_{jt}), \forall j \in J, \forall t \in T$	(55)
(36)	$\gamma^3_{jkt} \leq BM \times B^3_{jkt}, \forall j \in J, \forall k \in K, \forall t \in T$	(56)
	$\phi^{sugar}_{jkt} \leq BM \times (1 - B^3_{jkt}), \forall j \in J, \forall k \in K, \forall t \in T$	(57)
(39)	$\lambda^1_{ft} \leq BM \times Y^1_{ft}, \forall f \in F, \forall t \in T$	(58)
	$-(\sum_{j\in J} \phi^{coproduct}_{jft} - \varphi^{coproduct}_{ft}) \leq BM \times (1 - Y^1_{ft}), \forall f \in F, \forall t \in T$	(59)
(41)	$\lambda^2_{jt} \leq BM \times Y^2_{jt}, \forall j \in J, \forall t \in T$	(60)
	$-(\sum_{f\in F} \phi^{coproduct}_{jft} - W^{coproduct}_{jt}) \leq BM \times (1 - Y^2_{jt}), \forall j \in J, \forall t \in T$	(61)
(43)	$\lambda^3_{jft} \leq BM \times Y^3_{jft}, \forall j \in J, \forall f \in F, \forall t \in T$	(62)
	$\phi^{coproduct}_{jft} \leq BM \times (1 - Y^3_{jft}), \forall j \in J, \forall f \in F, \forall t \in T$	(63)

coordinates (i.e., latitudes and longitudes). This allows the user to consider one representative for each cluster, thus reducing the complexity of the problem. Second, the **SLM module** solves the SLM considering the clusters' representatives. Since the solution obtained at this stage does not necessarily maximize the leader's profit, a final step is required to **adjust the pricing decisions** considering the whole database.

5.1. Clustering module

As shown in Fig. 3, the user is involved before and after the clustering module. First, through a graphical user interface, the user must specify to the clustering module several parameters (e.g., the number of clusters respectively for corn farms, for depots' potential locations, for biorefineries and pig farms). The **clustering module** then generates candidate solutions for the cluster representatives using a clustering algorithm. In this paper, the K-Means algorithm for clustering is used, whose various parameters, such as the number of clusters, the maximum number of iterations, and the centroid initialization, must be set by the user. The use of the K-Means algorithm is motivated by the need to easily detect local geographic patterns by grouping data points according to their distances (Novianti et al., 2017). In addition, this algorithm is easy to implement and interpret, which is necessary for an interactive reoptimization approach. Various metrics (e.g., Silhouette index, Calinski–Harabasz index, and Davies–Bouldin index) enable the user to evaluate the clustering results and to choose the best configuration according to the nature of the data and the objectives of the analysis (Baarsch and Celebi, 2012). At the end of this step, the datasets of the corn farms, depots' potential locations, biorefineries, and pig farms can be reduced to cluster representatives. The graphical user interface presents a map showing the clusters and the user is prompted to select a representative to the SLM module a representative location for each cluster, as well as the optimization stopping criterion (the maximum resolution time in our case).

5.2. SLM module

Considering the clusters' representatives and the maximum resolution time set by the user, the SLM is solved using the solver BARON. Depending on the solution quality, the user can at this point adjust the maximum resolution time, and even restart the clustering step if necessary.

5.3. Price adjustment module

Since the pricing decisions made by the SLM module consider the clusters' representatives, they do not necessarily maximize the Leader's profit and they may not represent the optimal offers that the HUB can make to the followers. The price adjustment module provides the possibility to adjust the pricing decisions considering the whole database. This consequently leads to necessary adjustments in material flows as well.

The third step of the optimization process can be described as follows. The price adjustment module keeps some SLM decisions unchanged, namely depot locations, depot capacities, and production and supply levels. These decisions are parameters for three new Price Adjustment Models (PAM1, PAM2, and PAM3) derived from the original SLM. PAM1 (the biomass price adjustment model) adjusts the decisions $P^{biomass}_{jt}$ and $\phi^{biomass}_{ijt}$, respectively referring to biomass prices offered to corn farms and biomass sales at these prices. PAM2 (the sugar price adjustment model) adjusts the decisions P^{sugar}_{jt} and ϕ^{sugar}_{jkt}, respectively referring to sugar prices offered to biorefineries, and sugar sold at these prices. Finally, PAM3 (the coproduct price adjustment model) adjusts the decisions $P^{coproduct}_{jt}$ and $\phi^{coproduct}_{jft}$, respectively referring to coproduct

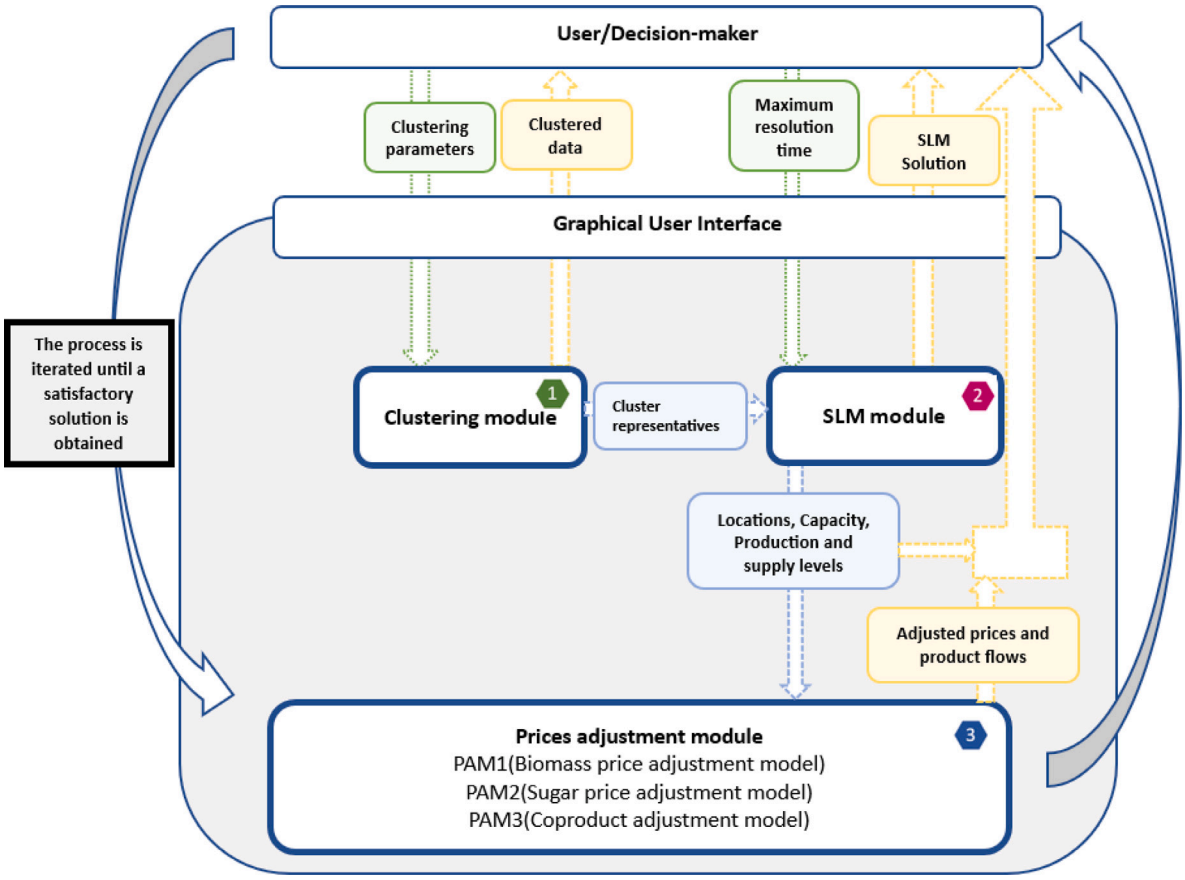


Fig. 3. A three-step optimization process.

prices offered to pig farms and coproduct sales at these prices. The formulation of these models is detailed in what follows.

For PAM1, two optimization levels are only considered from the SLM involving depots and corn farms. The following single-level model is obtained:

$$\max \Pi^J(P_{jt}^{biomass}, \phi_{ijt}^{biomass}) = -\sum_{t\in T}\sum_{i\in I}\sum_{j\in J} P_{jt}^{biomass}\phi_{ijt}^{biomass} - S^{biomass} \quad (64)$$

subject to constraints (12)–(14), (26), (28), (30)–(31) and (46–51).

For PAM2, two optimization levels are only considered from the SLM involving depots and biorefineries. The following single-level model is obtained:

$$\max \Pi^J(P_{jt}^{sugar}, \phi_{jkt}^{suagr}) = \sum_{t\in T}\sum_{k\in K}\sum_{j\in J} P_{jt}^{sugar}\phi_{jkt}^{suagr} + S^{sugar} \quad (65)$$

subject to constraints (15)–(17), (33), (35), (37)–(38), and (52–57)

Finally, for PAM3, two optimization levels are only considered from the SLM involving depots and pig farms. The following single-level model is obtained:

$$\max \Pi^J(P_{jt}^{coproduct}, \phi_{jft}^{coproduct}) = \sum_{t\in T}\sum_{f\in F}\sum_{j\in J} P_{jt}^{coproduct}\phi_{jft}^{coproduct} + S^{coproduct} \quad (66)$$

subject to constraints (18)–(20), (40), (42), (44)–(45) and (58–63).

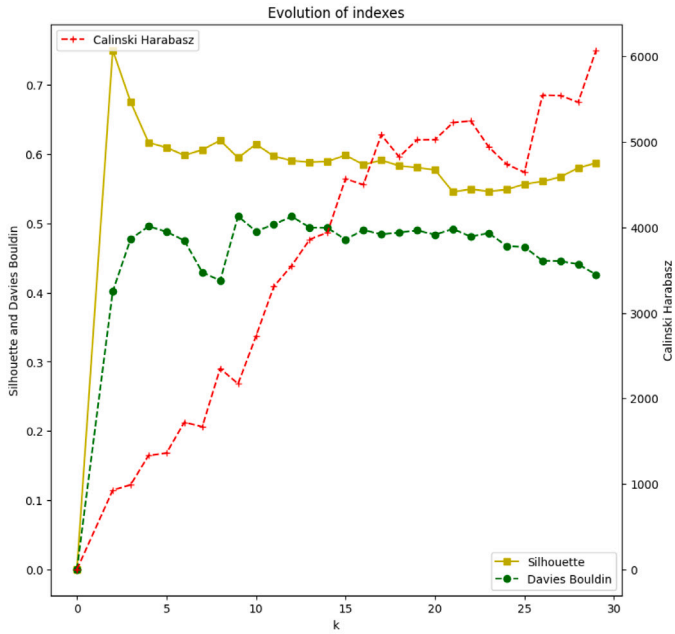
6. Experimentation and results

6.1. Data

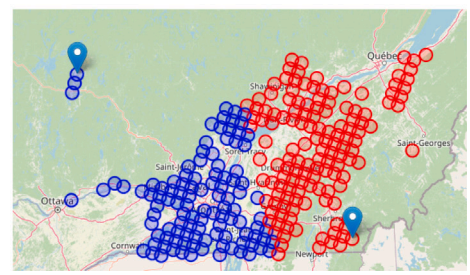
The case study addressed in this paper uses 5-year data on corn producers in the Province of Quebec. The database includes the locations of 247 corn farms and 286 pig farms, in addition to 395 potential depot locations identified. Each location is characterized by geographic coordinates (i.e., latitude and longitude), which enables the determination of a distance matrix between these locations. For simplicity's sake, this study considers a single biorefinery location. The theoretical availability of corn stover is provided by the Biomass Inventory Mapping and Analysis Tool (BIMAT) of Agriculture and Agri-Food Canada (Stumborg et al., 2008) while Quebec government data were used to represent the pigs' distribution in the territory (Ministère de l'Énergie et des Ressources naturelles et des Forêts, 2021). Cost and mass balance data are based on Lemire (2021) report. Table 7 presents the main parameters of the SLM. The maximum resolution time considered for the SLM is 8 h. The results obtained in each step of the optimization process are presented in what follows.

6.2. Results

In this subsection, the three-step optimization process proposed in Fig. 3 is tested for the real case study described above using a computer with these specifications: 8 GB RAM and an Intel Core i5 8th Generation CPU. In the first step, a single iteration of the interactive process was performed, beginning with an analysis of the clustering evaluation metrics as a function of the number of clusters for the **I** corn farms (Fig. 4(a)), **J** potential locations for processing depots (Fig. 5(a)), and **F** pig farms (Fig. 6(a)). Based on the evolution of the evaluation metrics in Figs. 4(a), 5(a), and 6(a), two clusters were chosen for **I**, four clusters for **J**, and two clusters for **F**. This decision was primarily driven by the observation that the Silhouette index reached its peak value when two clusters were selected for all actors. However, due to the limited biomass supply capacity at the depots, meeting the biorefinery's demand in year 5 requires a minimum of four depots. Since the Silhouette index decreases as the number of clusters increases,



(a) Clustering evaluation metrics for corn farms



(b) Clusters of corn farms

Fig. 4. Clustering of corn farms.

Table 7
Principal parameters of the SLM.

Parameter	Value	Unit
η^I	1	
μ	0.606	
α	0.316	
c^{fix}	476.97	\$/Ton
$tc^{fix,biomass}$	9.32	\$/Ton
$tc^{var,biomass}$	0.26	\$/Ton.Km
$tc^{fix,coproduct}$	22.63	\$/Ton
$tc^{var,coproduct}$	0.24	\$/Ton.Km
$tc^{fix,sugar}$	7.56	\$/Ton
$tc^{var,sugar}$	0.15	\$/Ton.Km
c^{sugar}	532.606	\$/Ton
$c^{coproduct}$	32.073	\$/Ton
q_{max}	10 112	Ton
$\varphi_t^{sugar}/t = 1..4$	17 340.66	Ton
$\varphi_t^{sugar}/t = 5$	34 681.32	Ton
$m_t^{biomass}$	2000	\$/Ton
$mc_t^{coproduct}$	100	\$/Ton
$m_t^{coproduct}$	0	\$/Ton
mc_t^{sugar}	1445.56	\$/Ton
m_t^{sugar}	0	\$/Ton

four depots were ultimately chosen to ensure demand fulfillment. Maps of the different clusters can be generated using software such as Power BI (see Figs. 4(b), 5(b), and 6(b)). Representatives were then set (see blue markers in Figs. 4(b), 5(b), and 6(b), one for each cluster) and used as inputs to the SLM. Additional iterations could be added by analyzing the results of this first iteration and adjusting the clustering of the data accordingly. For instance, the results could be contextualized, and weaknesses related to other aspects of the problem, such as access to road networks, could be identified. However, this was not done as it does not provide the reader with additional information about the optimization process itself.

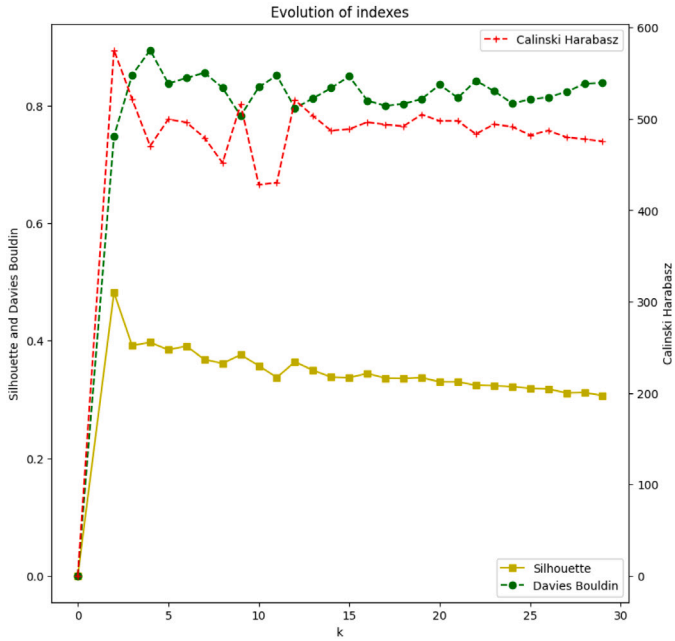
In the second step, the SLM was solved in a maximum of 8 h, using the parameters presented in Table 7. The SLM optimal decisions obtained in 745 min are shown in Table 8. According to the results in Table 8, a total of 99,698.64 tons of cellulosic sugar will be sold to the biorefinery over a period of 5 years. This quantity is expected to produce approximately 27,550,216.71 liters of bioethanol, assuming no losses, using the conversion ratio of 73 gallons per ton provided by Yue and You (2014). If this bioethanol is used to meet Quebec's low-carbon fuel mandates, it would replace approximately 275,502,167.1 liters of gasoline under the initial requirement of 10% bioethanol content. In the scenario where the 2030 requirement of 15% bioethanol is in place, it would replace about 183,668,111.4 liters of gasoline. This substitution would significantly contribute to the reduction of fossil fuel consumption and support the province's environmental goals. Finally, in the third step, price adjustments were made as follows.

6.2.1. Adjustment of biomass prices

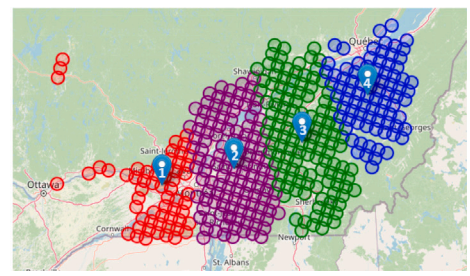
Fig. 7 presents the corn farms selected by PAM1. The adjusted prices provided by PAM1 and associated with the selected corn farms are presented in Table 9. In addition, Fig. 8 exhibits the quantities of biomass that will be sold by each corn farm to the different depots. PAM1 was successfully solved in 18 s, generating 40 intermediate solutions (since the solver used is based on local search algorithms), with the optimal one presented in this article. The adjustment model slashed the cost of biomass purchases by 63.94%, leading to a reduction of \$10,069,975.18 compared to the expenditure calculated when the SLM was solved. The profit of the HUB experienced a 16.22% rise, climbing from \$62,082,220 to \$72,152,195.20. This increase is explained by the fact that, following the biomass price adjustment (see Table 9), each depot is proposing prices lower than those recommended by the SLM module which considers cluster representatives (and not real data). The adjusted prices suggested by the depots only motivated the corn farms surrounding the depots to sell their agricultural residues as shown in Fig. 7.

6.2.2. Adjustment of coproduct prices

Fig. 9 shows the pig farms selected by PAM3. The adjusted prices provided by PAM3 and associated with the selected pig farms are presented in Table 9. In addition, Fig. 10 exhibits the quantities of coproduct that will be purchased by each pig farm from the different depots. PAM3 was successfully solved in 20 s, generating 42 intermediate solutions, with the optimal one presented in this article. The

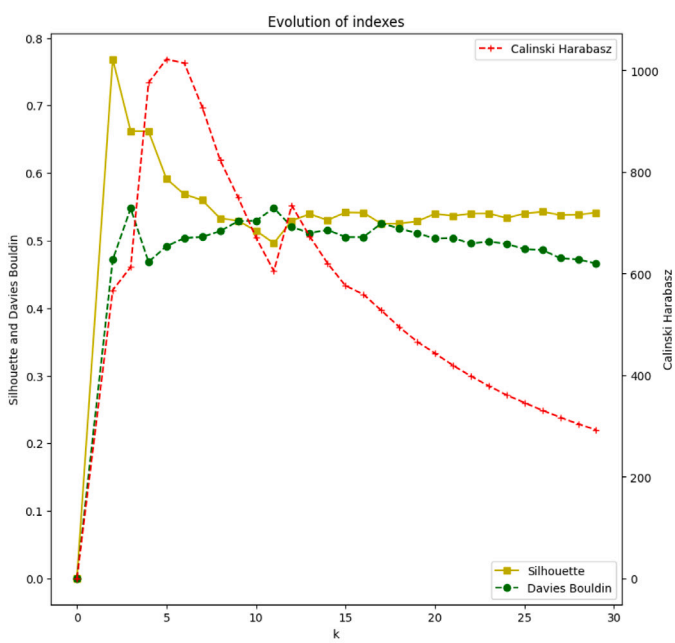


(a) Clustering evaluation metrics for potential locations

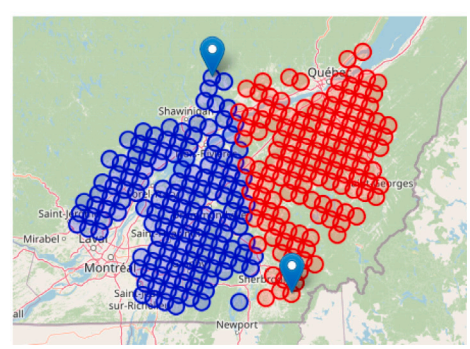


(b) Clusters of for potential locations

Fig. 5. Clustering of potential locations for processing depots.



(a) Clustering evaluation metrics for pig farms



(b) Clusters for pig farms

Fig. 6. Clustering of pig farms.

Table 8
Decisions of the SLM (Step 2).

Depots	Years 1 to 4 (Year5)						
	Capacity (Ton)	Biomass prices ($/Ton)	Biomass purchase(Ton)	Sugar prices ($/Ton)	Sugar sales (Ton)	Coproduct prices($/Ton)	Coproduct sales(Ton)
1	0(4345.32)	N/A(67.82)	0(13751.013)	N/A(1426.36)	0(4345.32)	N/A(21.45)	0(8333.114)
2	10112 (10112)	53.26 (53.26)	22875.506(32000)	1430.44(1430.44)	7228.66(10112)	36.81(36.81)	13862.557(19392)
3	10112(10112)	40.26(40.26)	32000(32000)	1416.55(1416.55)	10112(10112)	48.81(48.81)	19392(19392)
4	0(10112)	N/A(56.12)	0(32000)	N/A(1401.4)	0(10112)	N/A(36.33)	0(19392)

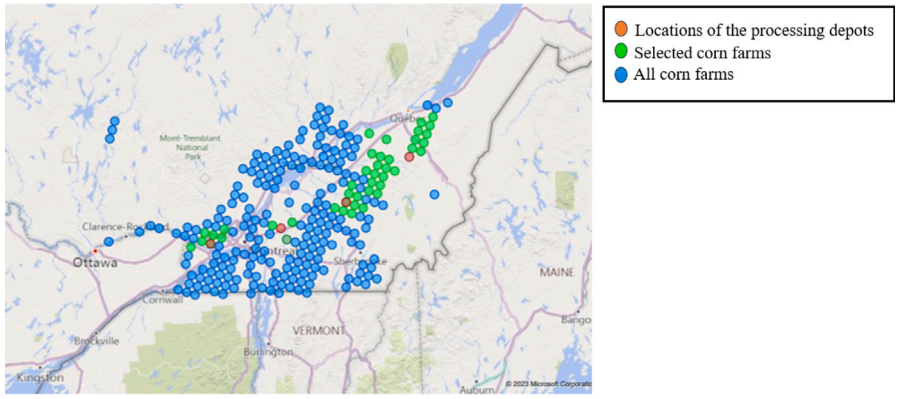


Fig. 7. Corn farms selected by the PAM1.

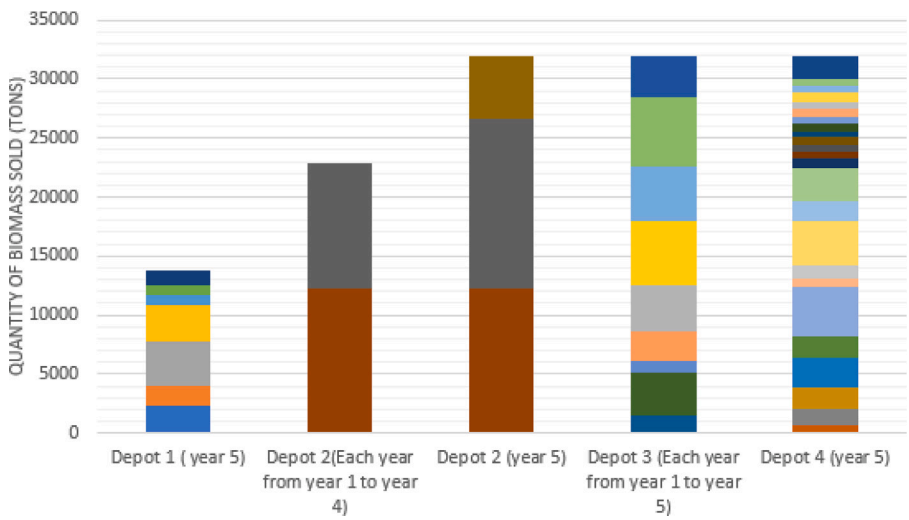


Fig. 8. Quantities of biomass sold by each corn farm to different depots.

Table 9
Comparison of biomass and coproduct prices determined by SLM and adjusted prices.

Depots	Years 1 to 4 (Year 5)			
	SLM biomass prices($/Ton)	Adjusted biomass prices ($/Ton)	SLM coproduct prices($/Ton)	Adjusted coproduct prices($/Ton)
1	N/A(67.82)	N/A(17.326)	N/A(21.45)	N/A(63.138)
2	53.26 (53.26)	14.462 (14.540)	36.81 (36.81)	72.834 (72.666)
3	40.26 (40.26)	17.154 (17.154)	48.81 (48.81)	69.642 (69.642)
4	N/A(56.12)	N/A(28.322)	N/A(36.33)	N/A(74.154)

adjustment model boosted coproduct sales revenues by 69.21%, resulting in a $5,793,604.024 increase compared to the amount calculated when the SLM was resolved. This led to an 8.02% increase in the HUB's profit, elevating it from $72,152,195.20 to $77,945,799.22. This increase is explained by the fact that, following the adjustment in coproduct prices (see 9), each depot is selling its coproduct at higher prices, exceeding what the SLM module suggests considering cluster representatives. The adjusted prices proposed by the depots only motivated the pig farms surrounding the depots to buy the coproduct from the depots as shown in Fig. 9.

The results presented above highlight the dynamics of the proposed DDM system and the effectiveness of coordination among the various actors in this industrial symbiosis. As shown in Table 7, sugar requested by the biorefinery in year 5 is higher than in years 1–4. Consequently, Table 8 shows that the biomass supply of depot 2 increased in year 5, compelling the depot to seek additional farmers. In addition, this depot increased its purchase prices, as evidenced by the adjusted biomass price value in Table 9. The same logic applies to the coproduct production level of depot 2 and its corresponding selling price: coproduct production increased in year 5. To sell this surplus quantity, depot 2 will reduce the coproduct selling prices in year 5 to attract more pig farms.

7. Discussion

In this paper, the value of industrial symbiosis was highlighted as a form of circular economy where the exchanges of waste and by-products between companies are economically viable. More specifically, the decision-making tool developed in this paper explicitly considers the distribution and sale of by-products generated by the treatment processes as a way to strengthen both business profitability and the reduction of the overall environmental footprint. Considering real-world assumptions, it was demonstrated that the developed tool can support the different decision-makers in the symbiotic bioethanol

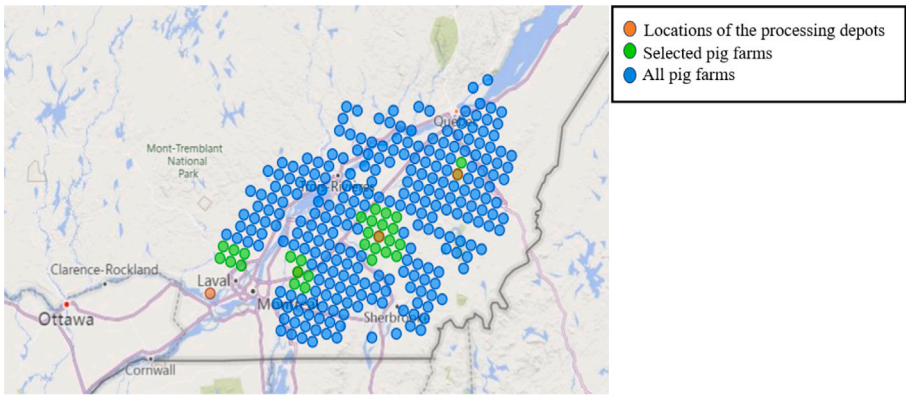


Fig. 9. Pig farms selected by the PAM3.

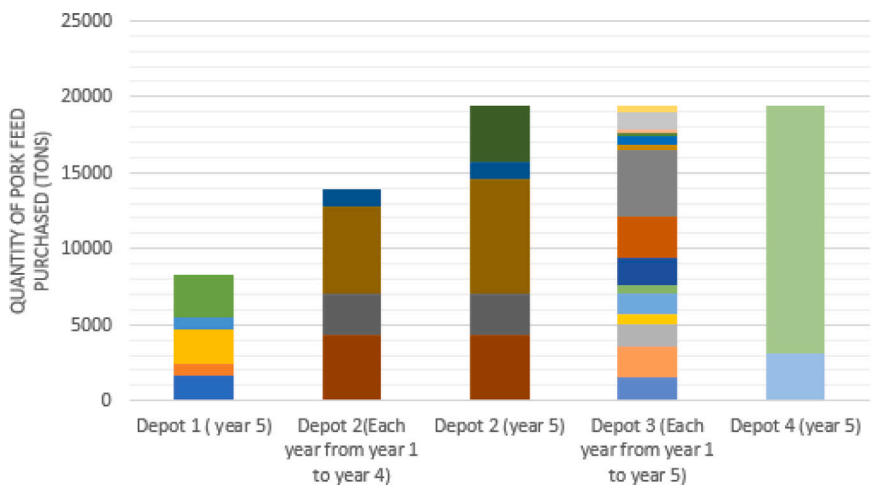


Fig. 10. Quantities of coproduct purchased by each pig farm from the different depots.

supply chain network. This network includes four actors: corn farmers (suppliers of corn residues), processing depots, biorefineries, and pig farms. The proposed tool optimizes the network design and coproduct pricing within a market equilibrium. On the one hand, the model allocates a crucial role to the HUB, which must make key decisions such as identifying the optimal locations for processing depots, as well as coordinating production plans and prices offered to suppliers and customers. On the other hand, considering the prices offered by the HUB and assuming a market equilibrium, the model provides the other actors with the optimal quantities of products to sell (for corn farms) or to purchase (for biorefineries and pig farms).

One of the advantages of the proposed tool is that it involves decision-makers and enables them to contribute to the design of the supply network and the selection of the most appropriate solution using the interactive reoptimization approach. In addition, the tool considers the mutual influences between the actors during decision-making and coordinates design and pricing decisions within the network. This approach also allows us to engage in network and beneficial exchanges, paving the way for a more efficient symbiotic network, and can be generalized for other sectors in which by-products could be dealt with within an industrial symbiosis context.

In addition to producing an eco-friendly product (bioethanol), the proposed industrial symbiosis valorizes by-products (corn residues) and coproducts (pig feed), reduces reliance on non-renewable resources, and limits environmental impacts. This case study demonstrates the economic balance that can be achieved. This can help managers overcome their fear of changes and losses, which is a common barrier to being part of an industrial symbiosis.

8. Conclusion

This paper proposes a novel distributed decision-making model for design and pricing decisions in a Biofuel Supply Chain Network in the Province of Quebec. As an industrial symbiosis, the involvement of four actors with diverse interests is proposed: corn farms, a HUB of processing depots, biorefineries, and pig farms. The problem is then formulated as a multi-period non-cooperative Stackelberg game under the Nash equilibrium assumption. As a leader, the HUB determines the depots' locations, production capacities, and supply and production levels. In addition, the HUB sets the purchase price of the biomass and the selling price of two products: the sugar offered to the biorefineries and the coproduct offered to the pig farms. The followers (i.e., each corn farm, each biorefinery, and each pig farm) independently optimize their own decisions regarding the quantities to sell or buy in order to maximize their profits.

To solve this problem, a DDM model is proposed and reformulated into a single-level model (SLM) using the Karush–Kuhn–Tucker (KKT) method. In addition, this article introduces a new resolution approach based on three modules that involve the user. The first module is the clustering module, which generates candidate solutions for cluster representatives using a clustering algorithm. The second module is the SLM module, where the SLM is solved considering the clusters' representatives and the maximum resolution time set by the user. The last module is the price adjustment module, which provides the opportunity to adjust pricing decisions and material flows, considering the real data, not only clusters' representatives. This approach is tested on a real case study in the Province of Quebec.

In the results section of this article, the place of the user was taken by choosing the clustering parameters and the maximum resolution time during the user-guided search. In this section, four clusters were chosen for the depots, two for the corn farms, and two for the pig farms. The representatives of these clusters were incorporated into the SLM module, which underwent a 445-minute runtime. The outcomes of the decision variables determined by the SLM are presented before the implementation of the price adjustment step. This step generates prices for various products and specifies the corn farms from which each depot will source, as well as the pig farms to which each depot will sell its coproduct. The comparison of the HUB profits both before and after the adjustment module is demonstrated by a profit increase of 25.55% after applying the price adjustments.

One limitation to consider is that when the optimization challenge takes on considerable proportions, it is common to resort to metaheuristics, although they do not guarantee an optimal solution. The resolution approach proposed in this article shares similarities with these metaheuristics in this respect, but it differs by actively encouraging the decision-maker to leverage their knowledge and intuition to incorporate additional constraints into the initial problem, with the aim of reducing its complexity. However, it is important to note that this approach does not guarantee the achievement of optimal solutions. While it does generate interest by allowing an easy representation of the problem and its solutions, as well as by involving the decision-maker in integrating relevant constraints, it cannot ensure the optimality of the generated solutions.

As far as the modification part of a current solution is concerned, this will be left to the company implementing this framework, to customize the adjustments according to their specific needs. It would be also interesting to consider the environmental impact of this symbiosis in the DDM model proposed for future research. In addition, more accurate resolution methods could be considered for the single-level model presented in this article. Also, it would be interesting to see the results with multiple biorefineries, unlike the case study presented in this article, which involves only one.

CRediT authorship contribution statement

Houssem Bouazizi: Writing – original draft, Validation, Software, Methodology, Formal analysis, Conceptualization. **Maha Benali:** Writing – review & editing, Validation, Supervision. **Jean-Marc Frayret:** Writing – review & editing, Validation, Supervision. **Rim Larbi:** Writing – review & editing, Validation, Supervision.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the authors used ChatGPT3.5 to improve readability and language. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

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Data availability

The authors do not have permission to share data.

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