Computers and Chemical Engineering 156 (2022) 107568

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Coordinated markets for furfural and levulinic acid from residual biomass: A case study in Guanajuato, Mexico

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ARTICLE INFO

Article history:
Received 5 March 2021
Revised 28 September 2021
Accepted 5 October 2021
Available online 13 October 2021

Keywords:
Biomass
Markets
Coordination
Levulinic acid
Furfural

ABSTRACT

Combustion of residual (waste) biomass represents an environmental hazard and a lost economic opportunity. The production of specialty chemicals provides a more attractive pathway to dispose of residual biomass; however, a problem that arises in recovering products from waste is that there are currently no well-established markets that bring together all stakeholders involved (e.g., biomass production, collection, transportation, and processing). In this context, coordination is essential as all the stakeholders in the supply chain (SC) depend on the revenue generated from the derived products. In this work, we propose a market coordination framework for the production of levulinic acid and furfural from lignocellulosic biomass (obtained from agricultural residues). Coordination brings a number of important economic benefits that would be difficult to achieve under existing markets (which are uncoordinated and based on peer-to-peer transactions). We demonstrate insights provided by our framework by using a case study for the State of Guanajuato in Mexico. Our results indicate that production of 330,000 tonnes per year of levulinic acid and 394,000 tonnes per year of furfural can be achieved. This constitutes 3% of the annual global demand for methyltetrahydrofuran. The SC is designed around a single biorefinery and the SC creates a total value of 3.57 billion USD per year and draws 64.65% of the available biomass supply. Our results also indicate that this market would avoid the generation of 850,000 tonnes of CO_2 annually (corresponding to a 34% reduction in emissions from the combustion of agricultural residues). As such, the deployment of such a market can bring both economic and environmental benefits.

1. Introduction

Combustion of residual biomass is a common practice worldwide that provides a simple pathway to manage agricultural waste (Yadav and Devi, 2018). However, the global CO_2 emissions arising from this management strategy are estimated to be 8.68 billion tonnes (Andreae, 1991). Of all anthropogenic emissions, biomass combustion is estimated to account for 40% of CO_2 emissions, 32% of carbon monoxide (CO), 20% of particulate matter, and 50% of polycyclic aromatic hydrocarbons (Kambis and Levine, 1996). In addition to such emissions, there are several other public health and safety concerns associated with biomass combustion (Lemieux et al., 2004):

- Smoke is released at or near ground level, resulting in acute exposure to concentrated pollutants in local populations.
- Combustion conditions can be difficult to control and this can lead to wildfires and inefficiencies (e.g., combustion can produce carcinogenic pollutants).
- Combustion can vaporize harmful chemicals (e.g., pesticides) and other greenhouse gases (e.g., nitrous oxide).

The World Bank argues that agricultural development is one of the most promising mechanisms for mitigating extreme poverty (Bank, 2020). For instance, the production of value-added chemicals from biomass could provide new opportunities for farmers to generate revenue from agricultural residues (creating a bioeconomy); moreover, the effective and controlled use of biomass residues can help mitigate environmental hazards associated with combustion. Since 2007, the number of commercial-scale production facilities for bio-based chemicals (biochemicals) has increased and the number of products reaching the market is also increasing. Moreover, the production capacity of the bio-based chemicals sector has grown faster than that of the fossil-based chemicals sector, with more than 8% annual growth (Popa and Volf, 2018).

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https://doi.org/10.1016/j.compchemeng.2021.107568

The OECD (Organization for Economic Co-operation and Development) argues that, by 2030, 30% of all chemicals will be biologically sourced (as chemical companies transition into biochemicals companies) (Popa et al., 2008). The bio-based chemicals market is poised to grow during 2020–2024 progressing at a CAGR of 11% during the forecast period (Research and Markets Ltd, 2021).

The concept of the biorefinery evolved during the late 1990s (Takkellapati et al., 2018); biorefineries are the renewable alternative to petroleum refineries. They are envisioned to utilize biomass (crops, grass, agricultural waste, wood, and municipal waste) as a renewable carbon feedstock to produce mainly biofuels (e.g., ethanol, biodiesel, bio-gasoline, hydrogen, methane) and chemicals (e.g., adhesives, coatings, paper, polymers) (Daoutidis et al., 2013a; Kelloway and Daoutidis, 2014; Daoutidis et al., 2013b). Five- and six-carbon carbohydrates present in lignocellulosic biomass can undergo selective dehydration, hydrogenation, and oxidation reactions to give high added value products such as sorbitol, furfural, glucaric acid, hydroxymethylfurfural, and levulinic acid (Egea et al., 2021; Walsh et al., 2012). Bio-product markets are dominated by a few companies, which are growing at an accelerated rate; for example, the GFBiochemicals company (located in Italy) is the world leading supplier of levulinic acid. The growth of this company has been steady (production of 1200 tonne/year in 2015 and 4200 tonne/year in 2016) and is envisioning the construction of a production plant with a capacity of 50,000 tonne/year (Scott, 2016; Levulinic Acid Market Share, 2021). Countries in the American continent (Mexico, the United States, and Canada) are among the main consumers of levulinic acid; as such, the implementation of these technologies in local regions could generate a positive impact in their economies. On the other hand, migration from oil-based technologies to bio-product-based ones is a reality. An example of this is the use of furfural as a raw material for the production of nylon 6-6 and other polymers, such as polyester. This technology was abandoned in 1961 by DuPont but is has been regaining interest in recent years (Anthonia and Philip, 2015; Isikgor and Becer, 2015). Therefore, it is important to show that countries with large reserves of lignocellulosic biomass begin a technological transition that can generate positive impacts on the economy and on the environment.

Establishing a *viable* biomass-based economy is difficult; this is because the associated supply chain (SC) involves a large number of stakeholders (e.g., farmers, transportation providers, biorefinery operators, and policy makers) and because the associated products have low margins. The biomass SC problem has been approached in a variety of ways, including the use of mixed-integer nonlinear programming (MINLP) models (Santibañez Aguilar et al., 2019; Santibanez-Aguilar et al., 2011; Akgul et al., 2014; Atashbar et al., 2016), mixed-integer linear programming (MILP) models (Ekşioğlu et al., 2009; Sawik, 2011; Denton et al., 2006), general disjunctive programming (GDP) (Zhang and Wright, 2014; Bai et al., 2012), and system dynamics (Saavedra Marroquin et al., 2018; Rendon-Sagardi et al., 2014). Most of these modeling studies focus on the conversion of biomass to biofuels or energy (not high-value chemicals). Moreover, these models assume that a single decision-maker operates the entire supply chain; in other words, this approach does not consider the welfare of individual stakeholders. In addition, such models do not take a market perspective of the problem; as such, these models do not reveal the inherent value of biomass and intermediate/final products. Consequently, they provide limited insights into potential economic bottlenecks that might hinder market implementation.

Game-theoretical models have been used for analyzing SCs (Li et al., 2019). Recently, we have proposed a coordinated market framework for managing multi-product SCs (Sampat et al., 2019). In such a setting, it is assumed that stakeholders (suppliers, consumers, and transportation/technology providers) bid into the market and a nonprofit entity (called an indepedent system operator-ISO) clears the market. This type of market is currently used for managing large electrical power networks around the world and provides a number of economic benefits (compared to uncoordinated markets operating through peer-to-peer transactions) (Blumstein et al., 2002; Nygren et al., 2010). Specifically, uncoordinated markets can run into circumstances where specific stakeholders are able to manipulate aspects of the market, resulting in inefficient outcomes (as manifested in California power crisis) (Joskow, 2001). Moreover, uncoordinated markets can lead to economic inefficiencies in complex systems (e.g., ineffective transport and transformation pathways). We have recently shown that coordinated markets prevent these issues and enable efficient production, transformation, and transportation of products (Tominac and Zavala, 2021). Moreover, we have shown that coordination does not interfere with the competitive nature of the stakeholders (coordination just accelerates convergence to an economic equilibrium). Coordinated market models are also useful in determining inherent values (prices) of products generated and to understand how revenue is distributed in the system (Tominac et al., 2021).

The biomass industry (especially the production of chemical building blocks) can help tackle social and environmental challenges. Additionally, this industry plays an important role in stimulating sustainable growth and creating competitive advantages in biomass-rich countries by creating industries that have close ties to rural and coastal communities (bolstering job creation in those areas). In this work, we propose a coordinated market framework for managing a biomass waste supply chain that produces specialty chemicals (levulinic acid and furfural), being the first time that a coordinated market approach has been used in an evaluation of these bio-blocks. This framework incorporates farmers (suppliers of biomass), transportation providers, processing systems required for the conversion of biomass to value-added products, and consumers of final products. The approach captures system-wide interdependencies and constraints that arise from transportation and bio-physico-chemical transformations of waste into diverse products. Our framework generates prices for each waste type and derived product at each geographical location, revealing the inherent value of intermediary and final products. We show that allocations and prices resulting from coordination satisfy fundamental economic principles. The proposed biomass SC is driven by the demand for specialty chemicals which we couple with a waste management service. Maximizing the social welfare of this supply chain simultaneously supports a valuable chemical industry and an environmentally-important waste management practice. We show that the proposed market provides a systematic framework to monetize environmental and health impacts, and quantifies the benefits associated with waste management. Moreover, prices reveal the true value of waste streams and derived products, and can be used to create incentives for investment and development of new technologies. Prices also capture spatial and temporal variations that help prioritize locations for investment in transportation, facility relocation, or seasonal waste storage. The framework can also be used by government agencies to understand and predict the effect of different regulation and incentive mechanisms. The proposed framework is also scalable, fostering transactions and interactions between large numbers of market stakeholders in urban and rural areas. We demonstrate our framework using a case study for the State of Guanajuato in Mexico. Our results indicate that production of 330,000 tonnes per year of levulinic acid and 394,000 tonnes per year of furfural are possible. This constitutes 3% of the annual global demand for methyltetrahydrofuran. Our results indicate that overall profit is maximized by an SC with a single centralized biorefinery; the associated market would create a value of 3.57 billion USD per year and utilize 64.65% of the available biomass supply. Importantly, the benefit to biomass suppliers is over 34 million USD annually, representing a potential revenue stream for regional farmers. Our results also indicate that, in addition to the economic value that our coordinated system would create, this system would avoid the generation of 850,000 tonnes of CO_2 annually (which corresponds to a 34% reduction in emissions from the combustion of agricultural residues). We present diverse scenarios to examine how profitability of all stakeholders is affected by economies of scale.

2. Coordinated market framework

We adopt the coordinated market framework presented in Sampat et al. (2019). In this framework, the geographical regions making up the market are represented by a set of connected nodes $\mathcal{N}$. The products exchanged in this market are denoted $\mathcal{P}$. Market stakeholders comprise a set of suppliers $i \in \mathcal{S}$, consumers $j \in \mathcal{D}$, transportation providers $l \in \mathcal{L}$, and transformation (technology) providers $t \in \mathcal{T}$. In our case study, products comprise different waste streams and derived chemicals. Transportation providers represent various alternatives (hauling, railway, pipelines, etc.) to move products between nodes.

Suppliers are defined $i \in \mathcal{S}$, with a location (node) attribute $n(i) \in \mathcal{N}$, and a supplied product attribute $p(i) \in \mathcal{P}$. Supplier i is willing to provide an amount $s_i \in \mathbb{R}_+$ to the market, not exceeding the amount $\bar{s}_i \in \mathbb{R}_+$, at the bid rate $\alpha_i^s \in \mathbb{R}_+$. Consumers are similarly defined $j \in \mathcal{D}$, with node $n(j) \in \mathcal{N}$, product consumed $p(j) \in \mathcal{P}$, consumption flow variable $d_j \in \mathbb{R}_+$ no more than the maximum of $\bar{d}_j \in \mathbb{R}_+$, with a bid of $\alpha_j^d \in \mathbb{R}_+$. As in the reference material, we use nested sets to simplify our notation, with $\mathcal{S}_{n,p} \subseteq \mathcal{S}_n \subseteq \mathcal{S}$ where $\mathcal{S}_n := \{i \,|\, n(i) = n\}$ (all suppliers located at a node n) and $\mathcal{S}_{n,p} := \{i \,|\, n(i) = n,\ p(i) = p\}$ (all suppliers located at node n supplying product p). Analogously, we have $\mathcal{D}_{n,p} \subseteq \mathcal{D}_n \subset \mathcal{D}$ for consumers.

Transportation providers $l \in \mathcal{L}$ move a product $p(l)$ from a node $n_s(l)$ (*sending*) to a node $n_r(l)$ (*receiving*). The transported amount is $f_l \in \mathbb{R}_+$, subject to the capacity $\bar{f}_l \in \mathbb{R}_+$, at the bid $\alpha_l^f \in \mathbb{R}_+$. The bid represents the transportation cost of moving material between nodes. To simplify notation, we define the sets $\mathcal{L}_n^{in} := \{l | n_r(l) = n\}$ (all transport flows into a node) and $\mathcal{L}_n^{out} := \{l | n_s(l) = n\}$ (all transport flows leaving a node). Similarly, we define subsets $\mathcal{L}_{n,p}^{in} \subseteq \mathcal{L}_n^{in} \subseteq \mathcal{L}$ defined $\mathcal{L}_{n,p}^{in} := \{l | n_r(l) = n, p(l) = p\}$ being the set of transport flows of product p entering node n. The sets $\mathcal{L}_{n,p}^{out} \subseteq \mathcal{L}_n^{out} \subseteq \mathcal{L}$ are defined analogously.

Transformation (or technology) providers $t \in \mathcal{T}$ have a node attribute $n(t)$, a set of consumed products $\mathcal{P}_t^{con} \subset \mathcal{P}$ and generated products $\mathcal{P}_t^{gen} \subset \mathcal{P}$. From among the products $p \in \mathcal{P}_t^{con}$ we define a reference product $\bar{p}_t$, in terms of which we define the technology flow $\xi_t \in \mathbb{R}_+$, the technology capacity $\bar{\xi}_t \in \mathbb{R}_+$, and the technology bid $\alpha_t^\xi \in \mathbb{R}_+$. The relative flows of consumed and generated products are defined by yield coefficients $\gamma_{t,p}$, where $\gamma_{t,\bar{p}} = 1$. Simplifying our notation we have the sets $(\mathcal{T}_{n,p}^{con}, \mathcal{T}_{n,p}^{gen}) \subseteq \mathcal{T}_n \subseteq \mathcal{T}$.

Market coordination proceeds via an independent system operator (ISO) who collects bidding information (including the bids α and the capacity parameters) and solves a dispatch (or market clearing) problem, determining the optimal allocations (s, d, f, ξ) and market prices. The ISO solution finds the optimal supply, demand, transportation pathways, and product transformations that maximize social welfare across the market network. In this context, social welfare is equivalent to the collective total profit allocated to the stakeholders. Stakeholders receiving a positive allocation are said to *clear*, and the sets $(\mathcal{S}^*, \mathcal{D}^*, \mathcal{L}^*, \mathcal{T}^*)$ are used to identify cleared stakeholders; i.e., $(\mathcal{S}^* := i \in \mathcal{S} | s_i > 0$. The market clearing process satisfies axioms of competitiveness, and results in prices that provide adequate remuneration to each cleared stakeholder.

2.1. Clearing formulation

The clearing problem is presented in (1) which illustrates the transfer of bidding information (bids $(\alpha^s, \alpha^d, \alpha^f, \alpha^\xi)$ and capacities $(\bar{s}, \bar{d}, \bar{f}, \bar{\xi})$) to the ISO from stakeholders. The ISO uses this information to solve the clearing problem, determining market allocations (s, d, f, ξ) and prices π, in doing so maximizing a social welfare objective (1a) subject to the clearing (conservation) constraints (1b). We note that the clearing constraint dual variable, $\pi_{n,p}$ is the nodal price of a product p at a node n. If the only set of feasible allocations is (s, d, f, ξ)=(0,0,0,0) we say the market is *dry*, otherwise the market *clears* (Fig. 1).

$$\max_{(s,d,f,\xi)} \sum_{j\in\mathcal{D}} \alpha_j^d d_j - \sum_{i\in\mathcal{S}} \alpha_i^s s_i - \sum_{\ell\in\mathcal{L}} \alpha_\ell^f f_\ell - \sum_{t\in\mathcal{T}} \alpha_t^\xi \xi_t \tag{1a}$$

$$\text{s.t.} \left(\sum_{i\in\mathcal{S}_{n,p}} s_i + \sum_{\ell\in\mathcal{L}_{n,p}^{in}} f_\ell \right) - \left(\sum_{j\in\mathcal{D}_{n,p}} d_j + \sum_{\ell\in\mathcal{L}_{n,p}^{out}} f_\ell \right) + \sum_{t\in\mathcal{T}_n} \gamma_{t,p}\, \xi_t = 0,\ \ (n, p) \in \mathcal{N}\times\mathcal{P},\ \ (\pi_{n,p}) \tag{1b}$$

$$0 \le s_i \le \bar{s}_i,\ \ i \in \mathcal{S} \tag{1c}$$

$$0 \le d_j \le \bar{d}_j,\ \ j \in \mathcal{D} \tag{1d}$$

$$0 \le f_\ell \le \bar{f}_\ell,\ \ \ell \in \mathcal{L} \tag{1e}$$

$$0 \le \xi_t \le \bar{\xi}_t,\ \ t \in \mathcal{T}. \tag{1f}$$

The market clearing allocations and prices determine the revenue and profit obtained by each stakeholder. Because each stakeholder strives to maximize its profit, market prices can be viewed as incentives that encourage stakeholder participation in various economic activities. These incentives can propagate through multiple stakeholders, encouraging cooperation to achieve profitable economic results. Through this lens, we examine bioproduct markets as a way of creating incentives that will encourage participation at each stage of the supply chain. Within our framework, we define four stakeholder-indexed price identities in (2) capturing the inherent value of economic activities in a supply chain. Identities (2a) and (2b) represent the price of supplying and consuming products, and are both equivalent to the nodal price for the corresponding product and the corresponding node. The price associated with transportation is defined by (2c) and is the difference between the nodal prices of some product at two different nodes. The technology price (2d) is the difference between the nodal prices of all output and input products for a technology located at some node. Importantly, the transport price demonstrates that a positive difference in nodal prices creates an incentive to move a product between nodes, while the technology price demonstrates that product transformation is incentivized when the combined value of outputs is greater than the combined value of inputs, accounting for yields. These relationships can be recovered either through revenue analysis (Sampat et al., 2019) or via the dual of the market clearing problem (Tominac and Zavala, 2021).

$$\pi_i := \pi_{n(i),p(i)} \quad i \in \mathcal{S} \tag{2a}$$

$$\pi_j := \pi_{n(j),p(j)} \quad j \in \mathcal{D} \tag{2b}$$

$$\pi_l := \pi_{n(l),p(l)} - \pi_{n'(l),p(l)} \quad l \in \mathcal{L} \tag{2c}$$

$$\pi_t := \sum_{p\in\mathcal{P}_t^{gen}} \gamma_{t,p}\pi_{n(t),p(t)} - \sum_{p\in\mathcal{P}_t^{con}} \gamma_{t,p}\pi_{n(t),p(t)} \quad t \in \mathcal{T} \tag{2d}$$

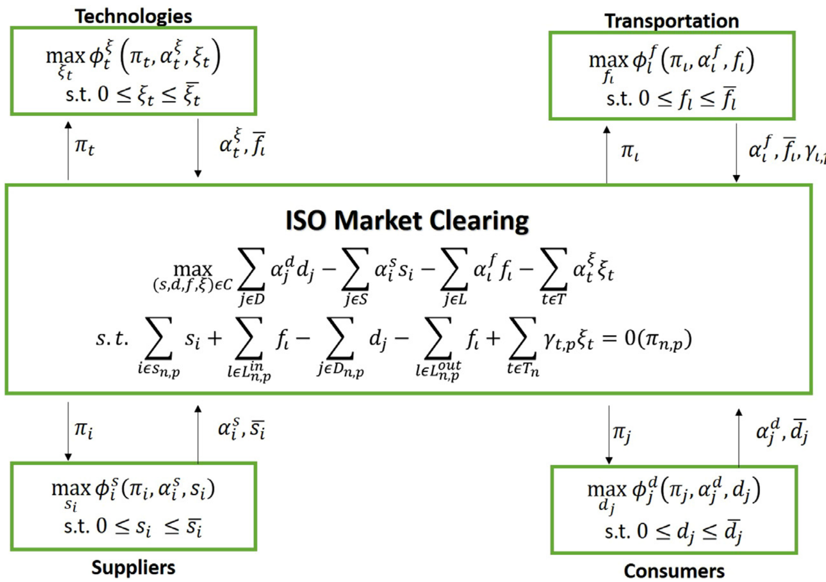

Fig. 1. Illustration of market coordination. Stakeholders share bidding information with the ISO, who solves the clearing problem, setting market prices and determining allocations. This procedure has the added effect of simultaneously maximizing each stakeholder objective.

Stakeholder profits are calculated as the difference between their revenue (a function of market prices and allocations) and their costs (determined from their bids, and the ISO allocations). Profit functions are presented in (3). We observe that profits all follow the same general pattern (profit is the difference between the stakeholder price from (2) and the corresponding bid, multiplied by the allocation) with the exception of consumers. In this case, the pattern is reversed, with the interpretation that a consumer's profit is money that is not spent; i.e., market prices below a consumer's bid creates profit for a consumer. We define $\phi := (\phi_s, \phi_d, \phi_f, \phi_\xi)$ to simplify notation.

$$\phi_i^s(\pi_i, \alpha_i^s, s_i) := (\pi_i - \alpha_i^s)s_i,\ i \in \mathcal{S} \tag{3a}$$

$$\phi_j^d(\pi_j, \alpha_j^d, d_j) := (\alpha_j^d - \pi_j)d_j,\ j \in \mathcal{D} \tag{3b}$$

$$\phi_\ell^f(\pi_\ell, \alpha_\ell^f, f_\ell) := (\pi_\ell - \alpha_\ell^f)f_\ell,\ \ell \in \mathcal{L} \tag{3c}$$

$$\phi_t^\xi(\pi_t, \alpha_t^\xi, \xi_t) := (\pi_t - \alpha_t^\xi)\xi_t, t \in \mathcal{T}. \tag{3d}$$

Market coordination satisfies important economic properties (Sampat et al., 2019). We summarize the properties here.

- Market coordination delivers prices π and allocations (s, d, f, ξ) maximizing collective profits ϕ and guarantees that profits are non-negative.
- Coordination delivers prices π and allocations (s, d, f, ξ) that represents a competitive economic equilibrium.
- Coordination delivers prices π and allocations (s, d, f, ξ) that satisfy revenue adequacy:
  $$\sum_{j\in\mathcal{D}} \pi_j d_j = \sum_{i\in\mathcal{S}} \pi_i s_i + \sum_{\ell\in\mathcal{L}} \pi_\ell f_\ell + \sum_{t\in\mathcal{T}} \pi_t \xi_t.$$
- The market satisfies the bounds: $\pi_i \geq \alpha_i^s$ for all $i \in \mathcal{S}^*$, $\pi_j \leq \alpha_j^d$ for all $j \in \mathcal{D}^*$, $\pi_t \geq \alpha_t^\xi$ for all $t \in \mathcal{T}^*$, and $\pi_\ell \geq \alpha_\ell^f$ for all $\ell \in \mathcal{L}^*$.
- If all transport provider bids α^f are all positive, then coordination will not emit an allocation with transport cycles.

Prices obtained with the proposed framework can also help create incentives and adjust biomass storage installation or intermediaries to avoid their application at certain times. In particular, under the proposed framework, prices are represented by the temporary value of agricultural waste. In countries such as Mexico, the agricultural waste market considers its use for the generation of energy through combustion and as a livestock feedstock. However, low prices encourage farmers to burn agricultural residues to start preparing the land for the next season. The prices obtained in the proposed framework reflect the associated costs and possible adjustments to the prices of agricultural residues and/or to identify optimal allocations for operations. The coordinated market framework can help to regularize the costs of cereals and thus have a strong impact on the agricultural sector. In addition, this framework can provide information to optimize the investment of funds for incentives associated with the management of agricultural residues and to incentivize the intervention of the private or government sector.

The framework can also be used to create incentives in the use of agricultural waste as raw material for other products. For example, in the United States, there was a key turning point when the Sustainable Fuels and Chemicals Act and the Biomass Research and Development Act that forced the Department of Energy (DOE) and the Department of Agricultura (USDA) to coordinate their efforts to develop biofuels, chemicals and energy from biomass in an efficient manner. As a result, the U.S. Congress awarded \$230 million USD to the DOE and the USDA to finance R&D activities in the field in question (Ochoa-Gómez, 2007). The incentive approach to avoid burning these agricultural wastes may involve discussions about the perception of various sectors, such as livestock, as some of these waste streams are used as livestock feed. Coordination can facilitate these discussions by providing information on how incentive generation can positively impact pollutant emission reduction and how changes can create new economic opportunities for stakeholders (e.g., farmers).

The proposed framework can also be synergized with environmental policy initiatives. For example, on 2008, the Law on Promotion and Development of Bioenergy (DOF, 2008) was introduced in Mexico to promote the production of supplies and raw materials, as well as the production, transport and marketing of bioenergy. Even though these incentives are focused on the development of bioenergy, the proposed coordinated market framework can also guide initiatives to the use of biomass for the generation of other value-added products.

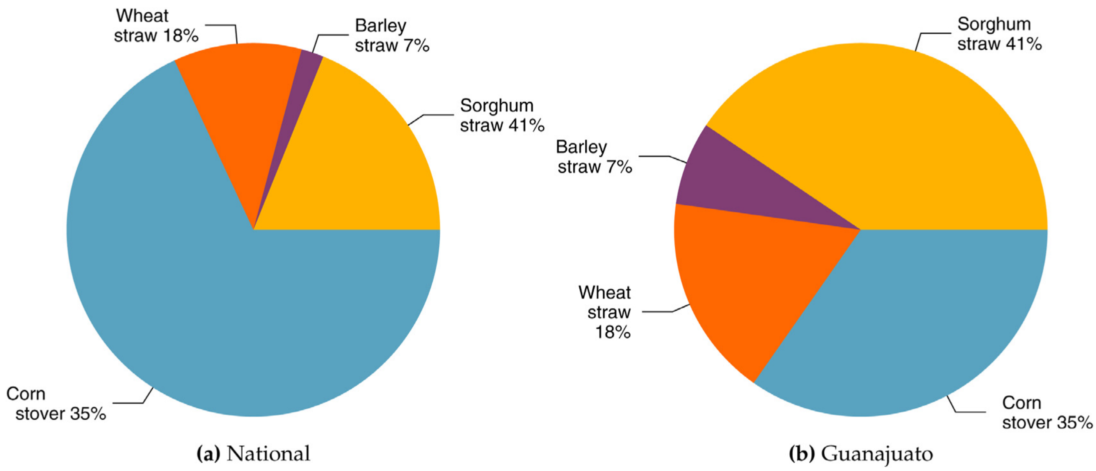

Fig. 2. Distribution of different agricultural waste products.

Table 1
Residue to crop ratio and residue price.

Main crop	Agricultural residue	Crop residue ratio (kg residue/ kg crop)	Agricultural residue price ($US/Mg)
Corn	Corn stover	0.825	18.33
Sorghum	Sorghum straw	1.425	14.97
Wheat	Wheat straw	1.835	16.67

3. Case study: biorefining agricultural residues in Guanajuato, Mexico

In Mexico, combustion of residual biomass accounts for 37% and 43% of all open fires (Ríos and Raga, 2018). Wildfires frequently occur in Mexico and Central America during the dry season (Crutzen and Andreae, 1991). Uncontrolled fires in 1998 were estimated to have covered an area of 13,962 km^2 in Mexico and Central America, leading to a declaration of air pollution emergencies in many cities (the resulting smoke traveled as far as Florida and North Dakota) (Ríos and Raga, 2018). At the same time, the Mexican government has continued to promote growth in the agricultural sector with the goal of promoting more efficient use of agricultural resources (CEDRSSA, 2020). Unfortunately, government regulations and incentives for biofuels programs have been insufficient to sustain market growth, and there has been limited investment in this sector. Bio-sourced specialty chemicals can provide economic incentives to achieve growth in this industrial sector. This would provide a market-based strategy (rather than reliance on government incentives) that can promote the more efficient use of biomass and the mitigation of emissions.

A study by the Mexican ministry of agriculture, livestock, rural development, fishing and food (SAGARPA) revealed that Guanajuato is the second largest producer of agricultural residues in Mexico (10.2% of the country total) SAGARPA (2015); Izquierdo et al. (2013). This makes Guanajuato a good candidate for the implementation of a bioproduct market. This region produces 3.8 million tonnes of agricultural residues annually, comprising 35% corn stover, 41% sorghum straw, 17% wheat straw, and 7% barley straw (Fig. 2). For this case study, we consider the three most abundant types of agricultural residues. Crop data was obtained from the Agri-Food and Fisheries Information Service (SIAP) (SIAP, 2019). SIAP provides crop production volumes for each municipality of Guanajuato, and we obtain the amount of biomass generated per crop using the residue ratio (McIlveen-Wright et al., 2013). We use agricultural residue prices reported by Santibañez Aguilar et al. (2019) (Table 1) as market bids.

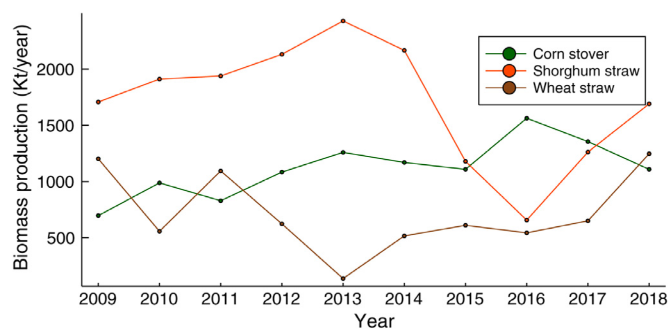

Fig. 3. Annual variations of biomass production in Guanajuato.

Table 2
Lignocellulosic biomass composition.

	Cellulose (%)	Hemicellulose (%)	Lignin (%)
Corn stover	35.0–39.6	16.8–35.0	7.0–18.4
Sorghum straw	32.0–35.0	24.0–27.0	15.0–21.0
Wheat straw	35.0–39.0	23.0–30.0	12.0–16.0

The coordinated market model was solved over 10 years (2009–2018) and each year was modeled as an individual instance. This approach allows us to account for variability associated with external factors such as droughts, pests, and floods. These factors influence the amount of biomass generated by each biomass supplier and therefore total chemical production, which means that there is some degree of uncertainty in their values (Fig. 3). Biomass composition was assumed to fall within the ranges reported by Isikgor and Becer (2015) and are shown in Table 2.

A couple of technology pathways were analyzed; the first pathway produces furfural along with methanol and other secondary products from hemicellulose. Conversion rates of 69% (furfural) and 17% (methanol) have been reported (Luo et al., 2019). Furfural is recovered from the reaction in liquid phase by steam stripping (to avoid degradation) and purified by double distillation. However, a yield of only 40–50% furfural is obtained after separation

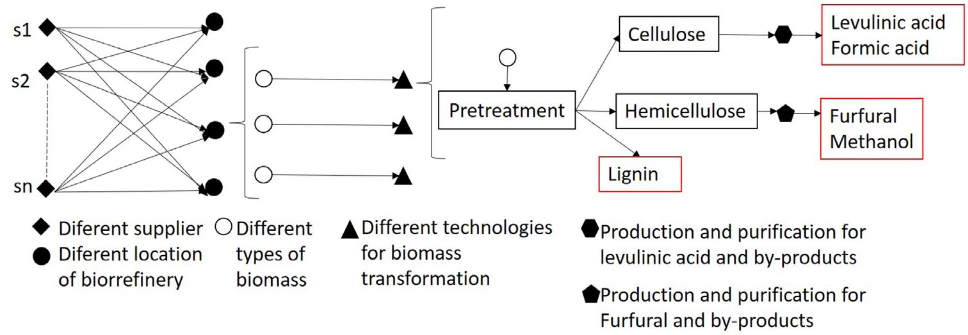

Fig. 4. Processing technology pathways for biomass.

Table 3
Biomass conversion factors to products and product prices.

Product	Conversion kg product/kg biomass			Price	
	Corn stover	Sorghum straw	Wheat straw	USD/tonne	Reference
Lignin	0.19	0.15	0.22	280	(Hodásová et al., 2015)
Ac. Levulinic	0.22	0.18	0.24	11,023	(Fitzpatrick, 2002)
Furfural	0.23	0.24	0.22	1700	(Montané et al., 2002)
Ac. Formic	0.08	0.07	0.09	600	(Pérez-Fortes et al., 2016)
Methanol	0.06	0.08	0.05	265	(Chong, 2019)

(Gürbüz et al., 2013; Yong et al., 2016). The second reaction route consumes cellulose and produces levulinic acid (49%), formic acid (18%), furfural (28%) and secondary products (Farone and Cuzens, 2000; Reunanen et al., 2013). Additionally, we assume that 97% can be recovered from levulinic acid after the purification process (Long et al., 2016). Biomass processing routes are shown in Fig. 4. We use the data to determine the conversion coefficients for each transformation provider (technologies) accounting for the different composition of each biomass feedstock (Table 2). Conversion factors have units of kg of product per kg of biomass and are shown in the Table 3. Feedstock prices (interpreted as supplier bid values) are also shown here.

Levulinic acid and furfural have been identified by the U.S. Department of Energy in the top 12 value-added products, owing to their use as components in methyltetrahydrofuran (MTHF) production (Mariscal et al., 2016). Specifically, MTHF can be blended into gasoline at 10% (No, 2019). Grand View Research estimated a potential demand of over 20 million tonnes of levulinic acid (a component in MTHF production) by 2020 (Research, 2015). Global furfural demand is estimated at 300,000 tonnes per year (Werpy et al., 2004; Montané et al., 2002). For our case study, we assume that up to 60% of the annual biomass is available for processing. This amount is selected by taking into consideration that biomass is also used as livestock feed. With the available biomass, we have estimated that the SC can produce 434,000 tonnes of levulinic acid per year and 487,000 tonnes of furfural, which represent 3.8% of the global demand for MTHF. At the proposed capacity, 9 million liters of MTHF fuel blend could be produced, corresponding to 128 millions average automobile fuel tanks per year.

Potential locations for biorefineries, biomass treatment, and production centers were strategically selected. The criteria for the selection were proximity to transportation infrastructure (highways and roads), provision of services for industries of each type, and proximity to available biomass (see Fig. 5). The locations correspond to industrial parks in the cities of Abasolo (R1), Celaya (R2), and Irapuato (R3), and Silao (R4). The industrial sector in the city of Leon is important but, due to frequent water shortages, was not considered (SAPAL, 2009).

Different locations and capacities of the biorefineries were considered in four scenarios. The scenarios are as follows:

- **Scenario 1.** Four biorefineries are installed, all having the same capacity.
- **Scenario 2.** Three biorefineries are installed, all having the same capacity. Generates four sub-scenarios (2a, 2b, 2c and 2d).
- **Scenario 3**. Two biorefineries are installed, all having the same capacity. Generates six sub-scenarios (3a, 3b, 3c, 3d, 3e and 3f).
- **Scenario 4.** One biorefinery is installed. Generates four sub-scenarios (4a, 4b, 4c and 4d).

These scenarios are used for analyzing the effect of economies of scale on total profit. The different scenarios considered are shown in Table 4. It is important to emphasize that each scenario is computed individually.

Regarding the production cost, it would be desirable to have information on technologies with the same Technology Readiness Level (TRL) and according to the capacities studied. However, the information concerning the process costs of the technologies to obtain the bio-blocks studied is scarce. In addition, the TRL method is not always the best alternative to compare technologies since it introduces certain biases that depend on the type of technology (Tomaschek et al., 2016). Additionally, the well-known six-tenths rule has extensively been used in the chemical industry to scale up (or scale down) the cost of technologies (Perkins, 1989). However, several works have shown that not all processes (or individual process components) follow this rule (Sánchez and Martín, 2018; Santibañez Aguilar et al., 2019). Production costs were obtained from literature studies in which economies of scales were explored (Cai et al., 2014; Gozan et al., 2018) and adapted to the required capacities. The cost estimate was therefore carried out by means of Eq. (4), where PC is the process cost (USD/Tonne) and BPC (Tonne/day) is the biomass processing capacity.

$$PC = 21113BPC^{-0.408} \tag{4}$$

Table 5 shows the capacity and cost for each technology proposed in each scenario; the proposed capacities were based on the available biomass. In our notation, tA1 consumes corn stover, tA2 consumes Sorghum, and tA3 consumes wheat straw.

Our model comprises 51 nodes, 1277 biomass suppliers, and 8 different products (raw materials and derived products) representing the 46 municipalities in Guanajuato and their production of agricultural residues for the years 2009–2018. Four possible tech-

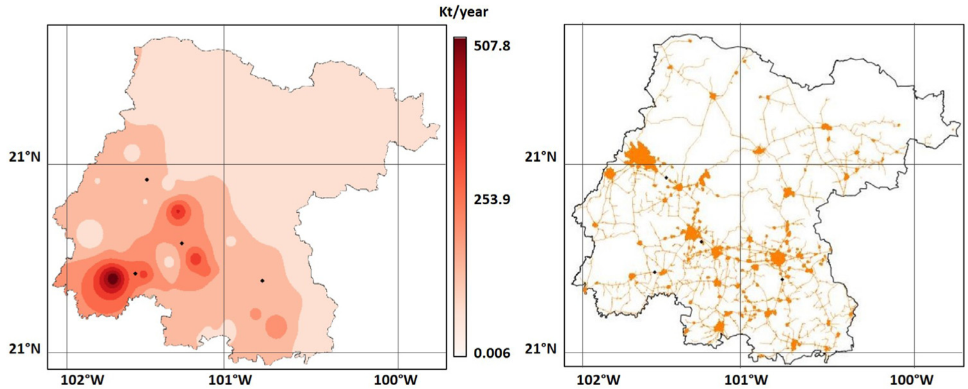

Fig. 5. Biomass variation in Guanajuato (left) and highway network and location of biorefineries (right).

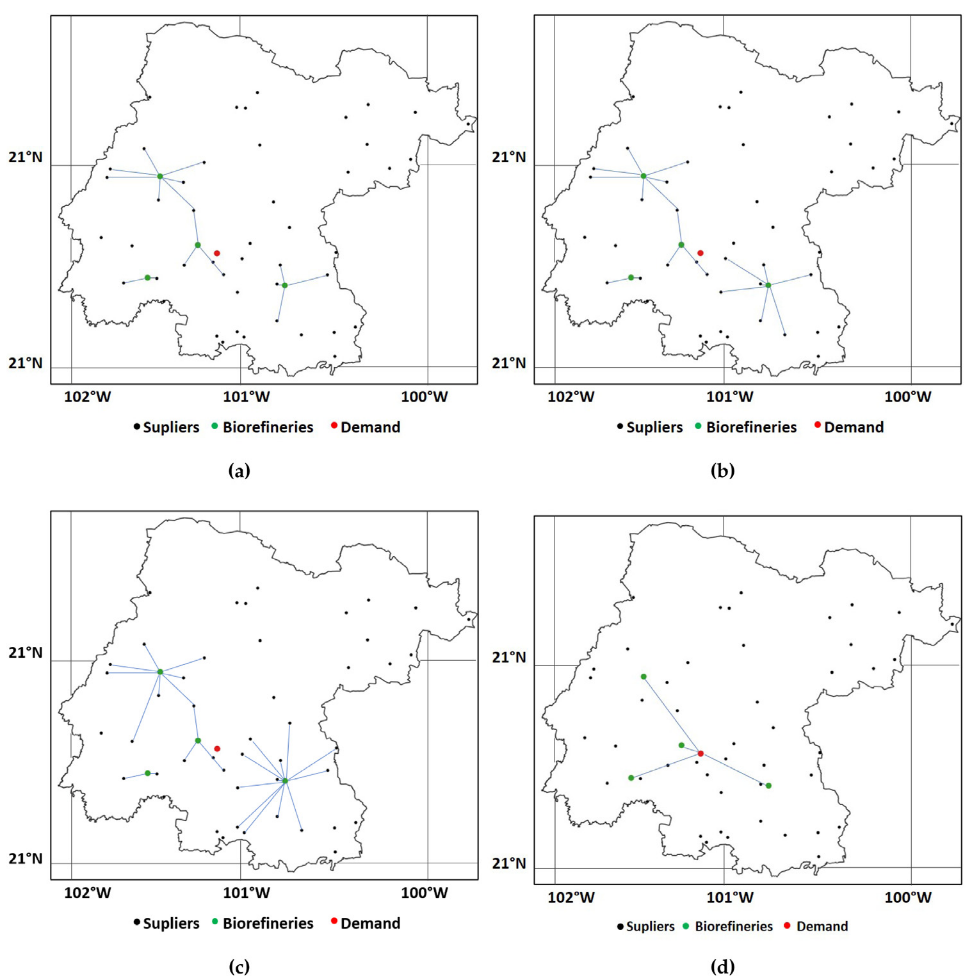

Fig. 6. Scenario 1. Cleared transportation flows for different biomass and derived products: A) Corn stover, B) Sorghum Straw, C) Wheat Straw and D) Derived products.

Table 4
Proposed scenarios.

	Scenario 1	Scenario 2				Scenario 3						Scenario 4			
Biorefineries included	1	2a	2b	2c	2d	3a	3b	3c	3d	3e	3f	4a	4b	4c	4d
R1	x	x	x	x		x	x	x				x			
R2	x	x	x		x	x			x	x			x		
R3	x	x		x	x		x		x		x			x	
R4	x		x	x	x			x		x	x				x

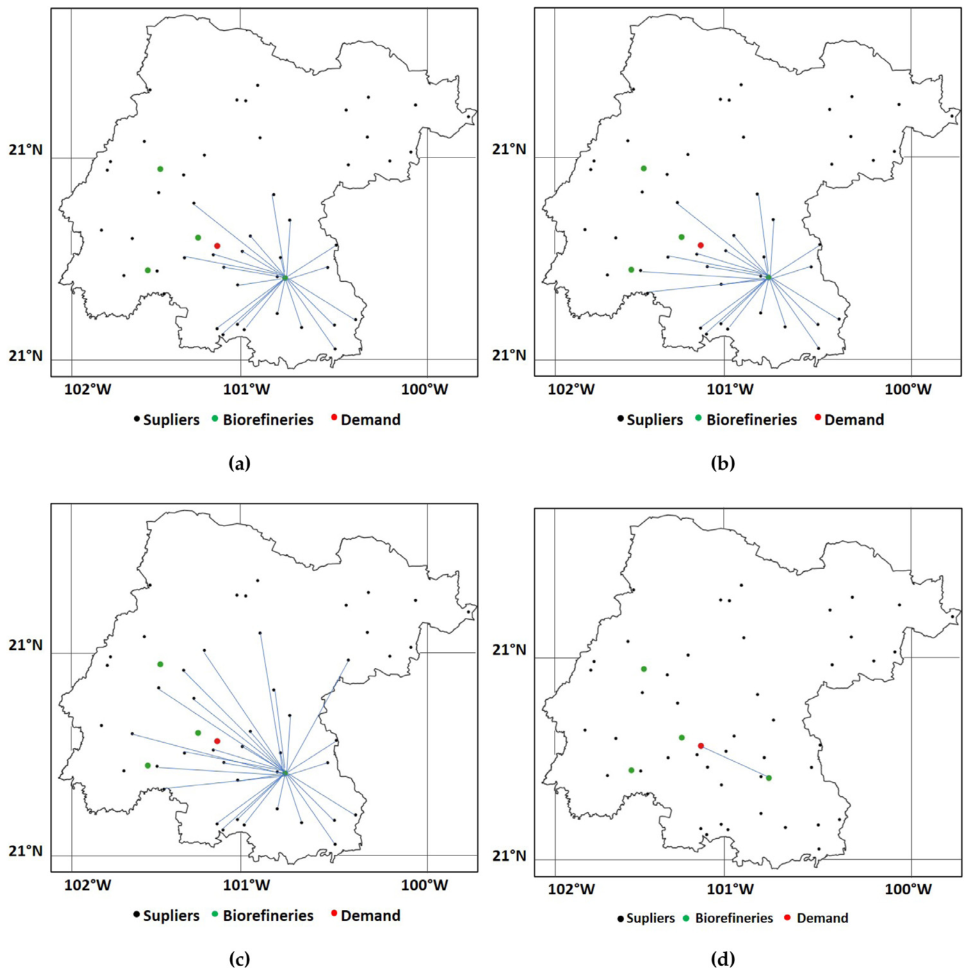

Fig. 7. Scenario 4b. Cleared transportation flows for different biomass and derived products: A) Corn stover, B) Sorghum Straw, C) Wheat Straw and D) Derived products.

Table 5
Capacities and production costs for different technologies.

	Technology	Capacity (tonne/day)	Production cost (USD/tonne)
Scenario 1	**tA1**	459	1719
	tA2	702	1430
	tA3	295	2160
Scenario 2	**tA1**	612	1512
	tA2	935	1288
	tA3	393	1853
Scenario 3	**tA1**	917	1297
	tA2	1403	1140
	tA3	590	1535
Scenario 4	**tA1**	1835	1068
	tA2	2806	984
	tA3	1180	1197

nology sites and a single point of demand for the products resulting from the transformation are modeled. The derived products obtained are fuel additives, so the demand node is the Ing. Antonio M. Amor refinery (operated by Pemex and which produces gasoline). For simplicity, we assume that transportation paths between nodes are linear; this gives rise to hundreds of thousands of possible paths. The clearing problem is a linear programming problem containing over 24,801 decision variables and 4860 constraints. This problem can be solved in 0.22 s using modern solution tools such as Gurobi 8.1.1. We used a processor Intel®Core^{TM} i5-6200 @2.30 GHz 2.4 GHz and 8 GB of RAM.

Table 6 shows the results of the different proposed scenarios. Since supply bids (biomass cost) are constant in all cases, we observe that all biomass available is consumed in every scenario. We explore economies of scale in our scenarios by reducing the total number of facilities but keeping the total processing capacity constant; as such, the facilities become larger as there are fewer of them. Economies of scale generally improve profit but not in all of our cases. In scenario 2, we reduce the number of biorefineries to three (increasing the capacity of these three, to keep the total constant) it is not possible to increase profit with respect to scenario 1a because the reduction in production cost is not enough to offset transportation costs, which increase as the number of biorefineries falls. In scenarios 3 and 4, it is possible to increase profit with respect to scenario 1a (by 15% and 32%, respectively) following from the reduction in production costs due to the economies

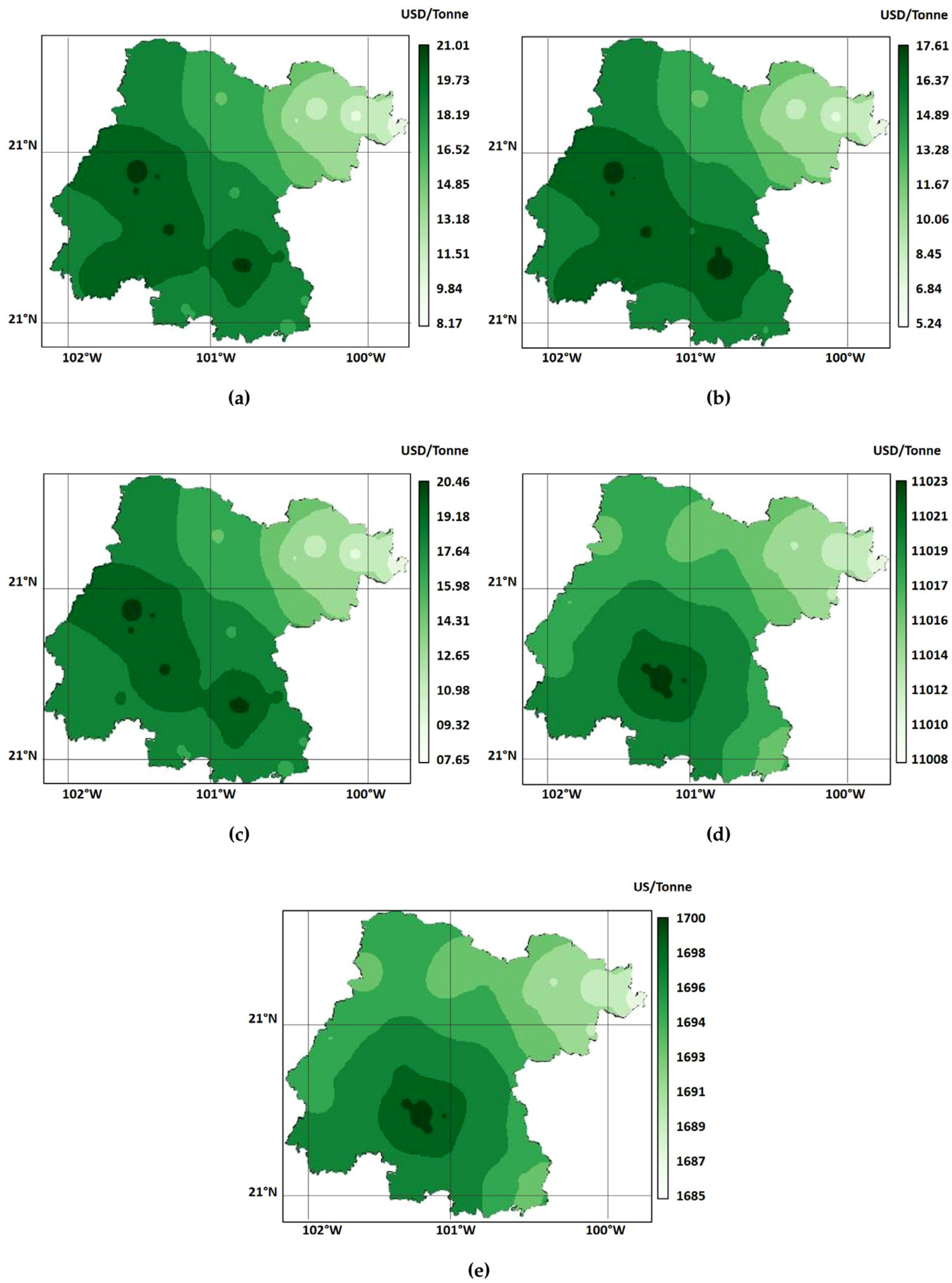

Fig. 8. Scenario 1. Clearing prices for different biomass and derived products: A) Corn stover, B) Sorghum Straw, C) Wheat Straw and D) Levulinic acid and E) Furfural. We can see geographical variations due to supply origin and transportation.

Table 6
Supply chain analysis for different scenarios.

Scenario	Total profit (Million USD/year)	Increase in profit (%)	Percentage of suppliers involved (%)	Supply cost (Million USD/year)
1a	2700		45.02	34.8
2a	2690	−0.51	44.24	34.8
2b	2690	−0.59	49.72	34.8
2c	2690	−0.54	38.99	34.8
2d	2690	−0.57	55.83	34.8
3a	3120	15.42	47.53	34.8
3b	3120	15.49	36.25	34.8
3c	3120	15.35	40.01	34.8
3d	3120	15.46	53.17	34.8
3e	3120	15.32	60.61	34.8
3f	3120	15.39	49.88	34.8
4a	3580	32.32	33.43	34.8
4b	3570	32.25	62.64	34.8
4c	3580	32.45	38.44	34.8
4d	3570	32.14	46.59	34.8

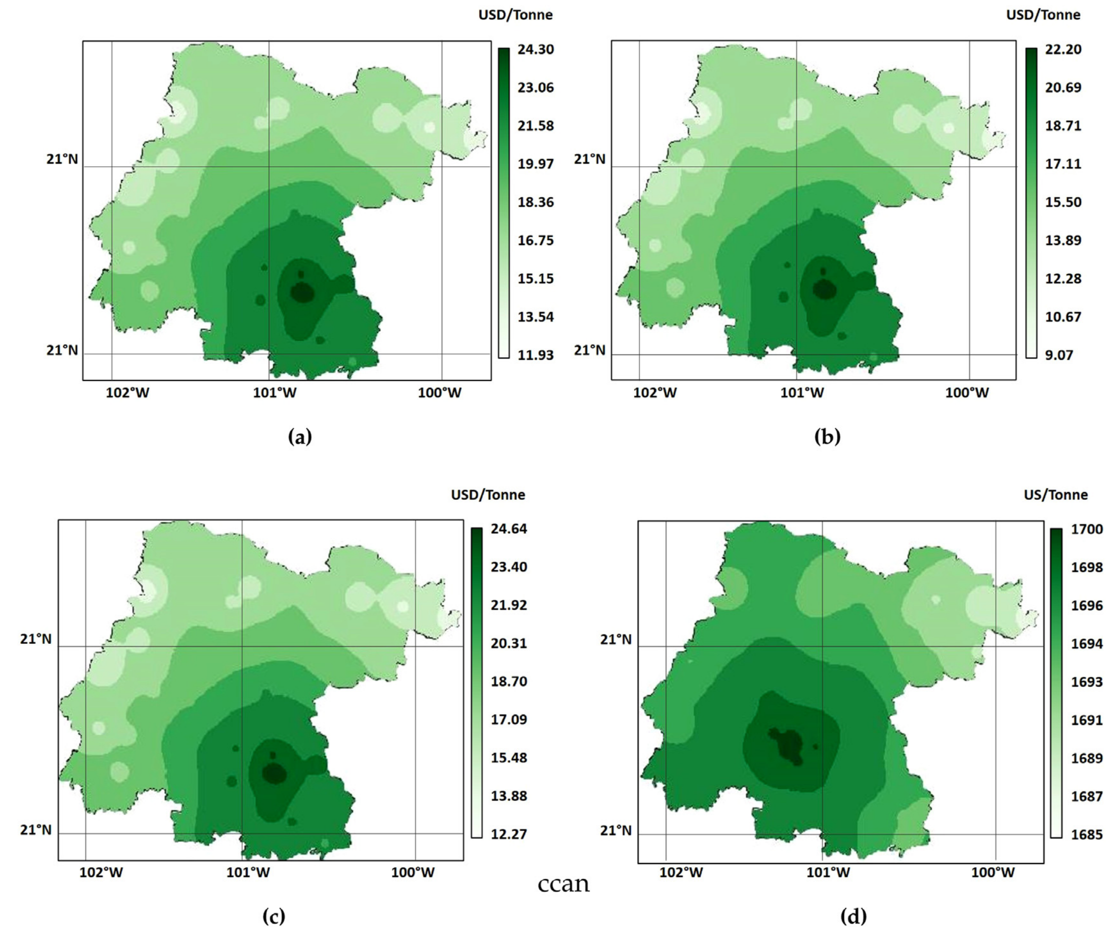

Fig. 9. Case 4b. Clearing prices in Guanajuato State for different biomass and derived products: A) Corn stover, B) Sorghum Straw, C) Wheat Straw and D) Levulinic acid and E)Furfural.

of scale. We desire a solution that not only maximizes profit but in turn involves the largest number of suppliers. From this perspective, scenario 4b appears to be the best option; achieving a total profit of 3570 million USD/year and involving 62.64% of the available suppliers. This scenario corresponds to the installation of a single biorefinery in the Celaya industrial park. We note that this scenario does not create the greatest total profit (but it is within 10 million USD/year of the best option); however, we select it because it includes the greatest number of suppliers (i.e., the required biomass is sourced from the largest number of farmers).

Since total demand was constrained to no more than 60% of the annual available biomass, spreading this amount over more farmers achieves two objectives: it distributes revenue streams to a the greatest number of stakeholders, and it reduces the amount of biomass obtained from an individual farm (again recalling that biomass has an additional role as livestock feed). We are interested in the fairness aspect of our solutions and so we explore an additional case. We limit each supplier to 60% of its biomass capacity. If the market achieves the same production rate as in 4b, then we expect that every supplier will be allocated this 60%. Re-solving this scenario, profit decreases by 7.48%, representing a loss of 267 million USD per year. In addition to the reduction in profits, only 96.31% of the suppliers participate in the market, demonstrating that transportation costs are prohibitive for some suppliers. These results can be used to provide guidelines to policymakers to build incentive programs for bioproduct supply chains. Importantly, this can potentially diversify biomass resources among multiple biofuels and energy economies. Market coordination maximizes total stakeholder profits (and no stakeholder loses money); this is an important aspect of our results, both for policymakers and in communicating supply chain strategies to farmers.

Figs. 6 and 7 present the transportation flows of the different biomass types and derived products from scenarios 1 and 4b, respectively. We choose scenarios 1 and 4b to demonstrate how the number of biorefineries installed influences supplier allocations, which is shown through changes in transportation flows. The location decisions have an important role in creating benefits for suppliers (farmers). In scenario 1, Fig. 6, the biomass flows (regardless of biomass type) are from suppliers close to the biorefinery. The number of suppliers is low since the proximity to municipalities with large production is sufficient to meet biomass demand.

In scenario 4b we observe that there is greater supply participation. Wheat residue flows in both cases are those involving a greater number of suppliers, this is because the municipalities produce wheat biomass in smaller quantities. In the case of non-participating (dry) municipalities, either transport costs are prohibitive or biomass of that type is not produced. Cleared transport flows of derived products flow from the biorefineries to the Pemex facility, as shown in Figs. 6D and 7 D.

Figs. 8 and 9 present the clearing prices for the different biomass types, and for levulinic acid and furfural for scenarios 1 and 4b, respectively. Similarly, the results of two scenarios are shown to visualize the effects generated by biorefinery location decisions. When there is a single point of demand, product prices show small variations, as in Figs. 8D,E, 9 D and E. However, when analyzing the prices of raw materials, we see that there is more

Table 7
Summary of economic results for Scenario 4b.

	(Million USD/year)
Profit	3570
Total revenue	5860
Total supply cost	34.80
Total transportation cost	12.30
Total technology cost	2240

variation due to competition between suppliers. It is important to note that scenario 4b has higher clearing prices for raw materials (Fig. 9A–C) than in scenario 1 (Fig. 8A–C). This shows that scenario 4b maximizes profit, and how it includes a higher percentage of suppliers than the other scenarios by creating a more favorable market for suppliers.

Table 7 shows the results of scenario 4b. The profit generated through the implementation of the coordinated market system is 3570 million USD per year, which is largely due to the price of levulinic acid. Total revenue was 5860 million USD/year, with a significant portion of this revenue used to cover process costs. Improvements in the production and purification processes for levulinic and furfural can reduce production costs and increase profits. The total cost of supply exceeds 34 million USD per year and the total cost of transportation is 12 million USD per year, which we interpret as a positive regional economic impact of more than 46 million USD per year. Furthermore, at a rate of 60% biomass consumption, the bioproduct market would avoid the emissions of 850,000 tonnes of CO_2 annually (Innes et al., 2000), which would correspond to 34% of the emissions from the burning of agricultural residues reported by the Institute of Ecology of the State of Guanajuato (IEE, 2005). This reduction in CO_2 emissions is considerable and would improve the air quality of the studied region. It is important to emphasize that the coordinated framework proposed can be implemented beyond this region and provides evidence of the potential of the use of biomass for the generation of products with high added value. The proposed coordination framework can be implemented in larger regions, handling other types of biomass, other types of technologies, and other types of products.

4. Conclusions

We presented a coordination market model to facilitate agricultural waste management in a scalable way by coordinating the exchange, transport and transformation of biomass into value-added products. The prices of waste and derived products in different geographical locations are obtained by solving a clearing problem that maximizes total profit and balances products throughout the region. Coordination resolves complex interdependencies between products and geographical relationships. We demonstrate that the system offers prices and allocations that satisfy the fundamental economic and efficiency properties. We also show that market coordination provides a systematic framework to monetize biomass in an unconventional way in the region, proposing an alternative for its use and thus avoiding its burning. Therefore, with the coordination of the market for the use of biomass, not only economic benefits would be generated, but also a reduction in CO_2 emissions and improvement of air quality. Market prices reveal the inherent value of waste streams and capture spatial variations that help prioritize geographical regions and reveal the need for investment in processing technologies, transportation, facility relocation, and seasonal storage. The proposed framework is scalable in the sense that it can provide open market access that encourages transactions between large and small stakeholders through the coordination infrastructure. We presented a case study with 4 scenarios, and observed the benefits of economies of scale through increasing profits. One of these scenarios achieves a total profit of 3570 million USD/year while including 62.64% of available supply. This scenario installs a single biorefinery in the study region. With the implementation of this coordinated market, the generation of 850,000 tonne of CO_2/year could be avoided, which would represent a 34% reduction in emissions from the burning of agricultural residues in the region. Our framework is a valuable first step towards the design of a bioproduct market in Mexico, which already has incentive programs for biofuels and bioenergy. Coordination frameworks will become increasingly necessary to provide reliable services as the human population grows and mobilizes and as resource availability becomes less predictable and more constrained. The proposed framework can potentially also be used to manage these more complex supply chain networks. As part of future work, we will also explore the use of market models that are uncoordinated and we will explore their economic properties.

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.

CRediT authorship contribution statement

Heriberto Alcocer-Garcia: Methodology, Formal analysis, Software, Writing – original draft, Visualization. **Juan G. Segovia-Hernandez:** Supervision, Writing – review & editing, Funding acquisition. **Eduardo Sanchez-Ramirez:** Writing – review & editing. **Philip Tominac:** Supervision, Writing – review & editing. **Victor M. Zavala:** Conceptualization, Supervision, Writing – review & editing, Funding acquisition.

Acknowledgments

Victor M. Zavala acknowledges funding from the U.S. Department of Agriculture (Grant 2017-67003-26055). Part of the work of Heriberto Alcocer-Garcia was conducted during a research visit at the University of Wisconsin-Madison (sponsored by CONACYT).

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