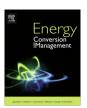
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Integrated decision making for the optimal bioethanol supply chain



Gabriela Corsano*, Yanina Fumero, Jorge M. Montagna

INGAR - Instituto de Desarrollo y Diseño (CONICET-UTN), Avellaneda 3657, S3002GJC Santa Fe, Argentina

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ABSTRACT

Bioethanol production poses different challenges that require an integrated approach. Usually previous works have focused on specific perspectives of the global problem. On the contrary, bioethanol, in particular, and biofuels, in general, requires an integrated decision making framework that takes into account the needs and concerns of the different members involved in its supply chain.

In this work, a Mixed Integer Linear Programming (MILP) model for the optimal allocation, design and production planning of integrated ethanol/yeast plants is considered. The proposed formulation addresses the relations between different aspects of the bioethanol supply chain and provides an efficient tool to assess the global operation of the supply chain taking into account different points of view. The model proposed in this work simultaneously determines the structure of a three-echelon supply chain (raw material sites, production facilities and customer zones), the design of each installed plant and operational considerations through production campaigns. Yeast production is considered in order to reduce the negative environmental impact caused by bioethanol residues. Several cases are presented in order to assess the approach capabilities and to evaluate the tradeoffs among all the decisions.

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1. Introduction

Nowadays, new perspectives have arisen around the firms integration resulting in new strategic challenges. Different entities or enterprises (suppliers, industrial facilities, warehouses, clients, etc.) integrate their activities in order to achieve global objectives. Generally, they do not belong to the same company, work in different trades and common actions affect their operations and performances. Previous approaches have pursued individual objectives, neglecting the combination of the units in the network. In this context, a supply chain (SC) is a common option where a set of units (e.g. suppliers, plants, warehouses, customers) makes a set of activities ranging from the purchase of raw materials to the transportation of finished products to clients. Thus, a first integration requirement can be posed respect to the links among the SC members.

In order to achieve an appropriate coordination, many decisions have to be taken into account. They can be classified into three levels regarding to their significance and the time period required in the planning horizon. Firstly, decisions about location, sizing and technology of plants and distribution centers are generally classified as strategic and they correspond to a planning horizon of several years. In a second level, procurement, product assignment as

well as distribution channel and transportation policy are considered as tactical decisions and they can be reviewed every few months. Finally, production planning, and the distribution of raw material, semi-finished and finished products in the supply chain are considered as operational decisions that are easily changed in the short term [1].

In general, previous works have addressed decision levels in hierarchical approaches in which SC design is first determined. SC design has been traditionally defined by determining the number and location of production plants, the sizing for each facility, and the flows among the different nodes of the network, pursuing economic objectives. Then, for each plant involved in the network, plant design decisions are made. Finally, planning decisions are determined using demand targets previously defined. On the other hand, there are few works dealing with SC design where first the plants are designed and then the surrounding SC. For example, in Baliban et al. [2] the synthesis and design of a thermochemical refinery is first solved and, then, in Elia et al. [3] the SC network of this kind of plants is designed. However, these hierarchical approaches do not consider any interactions between decision making levels and thus the SC design and planning decisions may result in suboptimal or even infeasible plant planning problems. Due to significant relations between decisions levels, it is necessary to consider the simultaneous optimization in order to determine the global optimal solution and to assess the tradeoffs among the different elements involved. Thus, a second integration

^{*} Corresponding author. Tel.: +54 342 4534451; fax: +54 342 4553439. E-mail address: gcorsano@santafe-conicet.gov.ar (G. Corsano).

Nomeno	clature		
Indices		NBC_{if}^{UP}	maximum number of batches of product i in the cam-
afer	alcohol fermentor	,	paign of plant f
b	batch	NN_f^{LOW}	left end of discretization interval of variable NN_f
bak	baker's yeast	NN_f^{UP}	rigth end of discretization interval of variable NN_f
bfer	biomass fermentor	Oper _{if}	operation cost coefficient for product i in plant f
С	customers zone	Q_{if}^{UP}	upper bound for the production of product i in plant f
cen cream	centrifuge centrifuged cream	QSC_s^{UP}	
d	points for discretizing the number of campaign repeti-	-	maximum amount of sugar cane discrete size m for semicontinuous units in stage j at
u u	tions	RF_{jmf}	plant f
dis	distillation	SF_{ij}	size factor of product <i>i</i> in batch stage <i>j</i>
et	ethanol	T_{ij}	processing time for product <i>i</i> in stage <i>j</i>
f	production plant	$tt_{df}^{"}$	d-th point obtained from the discretization of variable
i :	product		NN_f
J k	stage unit	VF_{jpf}	discrete size p for batch units in stage j at plant f
1	slot	α_{jf}	cost coefficient for batch units of stage <i>j</i> at plant <i>f</i>
m	discrete size for semicontinuous unit	β_{jf}	cost exponent for batch units of stage j at plant f conversion factor, i = tor, bak
M_{if}	number of available discrete sizes for a unit of semicon-	$ ho_i$	conversion factor, t = tor, bak
	tinuous stage j of plant f	Rinary V	/ariables
mol	molasses	ex_f	indicates if plant f is installed
n	number of batches of a product	NNC_{df}	specifies if the campaign of plant f is repeated tt_{df} times
p	discrete size for batch unit number of available discrete sizes for a unit of batch	,	over the time horizon H_f
P_{jf}	stage j of plant f	r_{jmf}	denotes if the units of semicontinuous stage j at plant f
r	raw material		have size m
S	raw materials site	v_{jpf}	denotes if the units of batch stage <i>j</i> at plant <i>f</i> have size <i>p</i>
tor	torula	x_{inf}	denotes if n batches of product i are processed in the campaign of plant f
vin	vinasses	Y_{bjklf}	denotes if b is assigned to slot l and processed in unit k
		- DJKIJ	of stage <i>j</i> in plant <i>f</i>
Sets		Z_{jkf}	specifies if unit k of stage j at plant f is employed
BI_i	batches of product <i>i</i> proposed for the production cam-		
EB_i	paign batch processing stages used for producing <i>i</i>		ous variables
ES_i	semicontinuous processing stages used for producing <i>i</i>	ANB	annual net benefit
SR_{if}	available discrete sizes for units of semicontinuous	B_{if}	batch size of product <i>i</i> at plant <i>f</i>
9	stage j in plant f	CTC_f	cycle time of the campaign of plant f represents the bilinear term z_{jkf} v_{jpf}
SV_{jf}	available discrete sizes for units of batch stage j in plant	e _{jkpf} ee _{jkmf}	represents the bilinear term $z_{jkf} r_{jmf}$
	f	INSC	installation cost
		INVC	investment cost
Paramet		IS	income for sales
Cap ₁	Capacity of molasses truck truck capacity for transporting product <i>i</i>	NB_{if}	total number of batches of product i processed at plant f
Cap _i CCF	capital charge factor	NDC	in the time horizon H_f
inc _f	fixed cost for plant f installation	NBC_{if}	number of batches of product i included in the campaign of plant f
Cfuel	fuel cost	NC_f	number of times that the campaign of plant f is cycli-
CSCane _s	sugar cane procurement cost, per mass unit, in site s		cally repeated over the time horizon H_f
CTC_f^{UP}	upper bound for variable <i>CTC_f</i>	OC	operating cost
CTIFC _{ifc}	transportation cost, per mass unit, of final product i	Q_{if}	amount of product i produced in plant f
3	from plant f to customer c	QC_{ifc}	amount of product i sent from plant f to customer zone c
CTRAW _{s1}	f transportation cost, per mass unit, of raw material r	QM_s	amount of molasses produced at site s
D.	from site s to plant f	QR_{sf}	amount of molasses sent from site s to plant f
D _{ij}	duty factor of product <i>i</i> in semicontinuous stage <i>j</i> distance between raw material site <i>s</i> and plant <i>f</i>	R_{jf}	size of a semicontinuous unit in stage j of plant f
dist1 _{sf} dist2 _{fc}	distance between plant f and customer zone c	ResC	disposal cost
DM_{ic}^{LO}	minimum demand of product i from customer zone c	SCC	sugar cane cost
	_	TF _{jklf}	final processing time of slot <i>l</i> in unit <i>k</i> of stage <i>j</i> at plant <i>f</i>
DM_{ic}^{UP}	maximun demand of product <i>i</i> from customer zone <i>c</i>	TI_{jklf}	initial processing time of slot l in unit k of stage j at plant f
fc_f	conversion factor that indicates the kg of molasses required to produce one L of ethanol at plant f	TRANC	transportation cost of raw materials from sites to plants
H_f	time horizon for plant f		and of final products from production plants to
K _{if}	maximum number of identical parallel units that can be		customer zones
JJ	allowed at batch stage j of plant f	u_{ijmnf}	variable that denotes to Q_{if} if the binary variables r_{jmf}
L_{kjf}	number of slots postulated for unit k of stage j in plant f		and x_{inf} simultaneously take the value 1
I			

 V_{jf} size of a batch unit in stage j of plant f W_{ijpnf} variable that denotes to Q_{if} if the binary variables v_{jpf} amount of discarded centrifuged cream v_{ijpnf} amount of discarded vinasses v_{ijpnf} and v_{inf} simultaneously take the value 1 v_{ijpnf} represents the cross product of variables v_{ijpnf} v_{ijpnf} and v_{inf} simultaneously take the value 1 v_{ijpnf} represents the cross product of variables v_{ijpnf}

requirement can be posed, considering the links among the decision levels.

Moreover, bioethanol, in particular, and biofuels production, in general, present specific requisites. A multidisciplinary approach is required where new sustainability considerations are now closely dealt with economic and operational objectives, defining a new integration requirement.

Taking into account these strong integration necessities, appropriate tools must be considered in order to adequately assess the impact of the different proposed solutions. Mathematical modeling is a suitable approach to represent the tradeoffs among the different involved elements and achieve optimal decision making. In this way, a new mathematical formulation is proposed in this work, where the different perspectives and requirements of the involved units and decision levels are simultaneously considered. Although a simple process description is adopted, the suggested approach allows appraising its impact on the bioethanol production management.

In the last years, there have been some efforts to integrate decisions in SC optimization, particularly at strategic and tactical levels. For example, a new mixed integer linear program (MILP) was introduced by Lainez et al. [4] for the optimal design and planning of SC. The proposed approach integrates strategic and tactical decisions increasing the computational complexity but the authors highlight that significant improvements can be achieved when decisions are combined. Reverse flows were introduced by Amaro and Barbosa-Póvoa [5] in order to pose a new formulation for the sequential planning and scheduling of SC. Planning and scheduling decisions of a chemical SC, as well as financial management issues, were approached by Guillén et al. [6]. A mixed-integer nonlinear program (MINLP) model was proposed by You and Grossmann [7] where inventory optimization and SC network design under demand uncertainty are simultaneously taken into account. You et al. [8] posed a multi-period MILP formulation for the simultaneous sizing, production, and distribution planning for a system considering diverse locations for the production facilities. Different product families can be produced according to the potential capacity modifications in the production facilities.

In the last decade, growing ethanol production as a source of renewable energy, has increased studies on ethanol SCs. Among biofuels, bioethanol is currently considered the most appropriate solution for a short-term gasoline substitution [9]. Several authors have addressed the design and planning of ethanol SC through mathematical modeling and optimization, and due to the environmental impact caused by this production, sustainable aspects were also considered in many works. An et al. [10] presented a detailed review about biofuel and petroleum-based fuel SC, and they highlight that no available models integrate biofuel SCs in all decision levels. In Grossmann and Guillen-Gosalbez [11] a general overview of process synthesis and supply chain management (SCM) formulation considering environmental criteria is provided. They highlighted the main optimization models presented in the literature, including the handling of uncertainty and the multi-objective optimization of economic and environmental objectives. Recently, Nikolopoulou and Ierapetritou [12] presented a review of the relevant research on sustainable chemical processes focusing on green SC, energy efficiency and waste management. Zamboni et al. [13] formulated a multiobjective model for optimizing the design of the corn-based ethanol SC in northern Italy. Das-Mas et al. [14]

proposed a dynamic MILP model for the optimal design and investment capacity planning of an ethanol SC under price uncertainty. They applied the approach to an Italian study case in order to assess the economic performance and risk on investment of the entire biomass-based ethanol SC. In Giarola et al. [15] the strategic design and planning optimization of bioethanol supply chains through first and second generation technologies are addressed. A MILP model was proposed in order to optimize both environmental and economical objectives jointly. The formulation serves as a guide for taking decisions and investments through a global approach. Kim et al. [16] presented a MILP model where fuel conversion technologies, facility capacities, biomass supply locations, and the transportation between the different SC nodes are simultaneously selected. They considered distributed and centralized networks and compared them in terms of their profits and robustness, according to demand variations. Mele et al. [17] formulated a multi-objective MILP for the simultaneous optimization of economic and environmental performance of an Argentinean sugar/ ethanol supply chain. They analyzed several tradeoffs between economic and environmental measures of the network. In a later work, Kostin et al. [18] incorporated uncertainty in the demand to the previous work. They proposed a multi-scenario MILP problem that includes the capacity expansions of the plants and deports over time and the associated planning decisions. The strategic design of a hybrid first/s generation ethanol supply chain was addressed in Akgul et al. [19]. The model, formulated as a MILP, addresses sustainability issues such as the use of food crops, land requirements of second generation crops and competition for biomass with other sectors. Grisi et al. [20] present a MILP formulation to solve the short term operation of biorefineries from sugarcane industry. Cucchiella and D'Adamo [21] analyze the specific characteristics of SC of renewable energies, considering the relationships among environmental, economic and social aspects.

On the other hand, all the previous mentioned works have considered the design and planning of SC without taking into account process performance models for the involved facilities in the SC.

A general MILP model was formulated by Corsano and Montagna [22] for the optimal SC and embedded plants design. That approach integrates strategic decisions of the SC and the multiproduct batch plants, as the selection of SC nodes and flows between them, plant configuration and sizing, etc. In this way, the simultaneous resolution of both problems allows to evaluate the several tradeoffs among different decision variables that cannot be assessed using sequential approaches. The authors show that there are tradeoffs between involved decisions and those problems should be simultaneously solved. In a later work [23], a Mixed Integer Non Linear Programming (MINLP) optimization model for the optimal sustainable design and operation of the ethanol SC from sugar cane is presented. A detailed model for the ethanol plant design was included in the overall SC model in order to simultaneously attain plant and SC designs. Similar conclusions were obtained for the case of bioethanol production. These previous approaches were focused on design models. Even though they included more detailed models in order to analyze the links between SC and plant decisions, they do not consider operations management issues. For example, both works assume that the involved plants operate using the simplest scheduling policy: single-product campaign mode. In this case, only one product is considered in the campaign which is finished when its demand is fulfilled. Obviously, this assumption allows obtaining simplified models. Nevertheless, from the operational and commercial perspectives, this policy is unrealistic since, for example, enormous stocks should be maintained to support this proposal, which can be impracticable when perishable products are considered.

Fumero et al. [24] presented a MILP model for simultaneous design and detailed production planning of a semicontinuous/ batch plant for ethanol and derivatives production. Their approach establishes the optimal plant configuration (unit dimensions, units duplication) and the production planning using mixed product campaigns (MPC) (number of batches of each product in the campaign and its sequencing) to minimize the investment cost fulfilling the required demands. In this case, a campaign is composed by several batches of different products which are produced in the plant following a sequence which is cyclically repeated over the time horizon. This solution is appropriate in a stable scenario. Although this assumption cannot be assured for all the industries for a long term context, this is suitable supposition for the ethanol production. Thus, estimation for the production flows can be calculated, and their impact over several decisions: stocks, transportation, supplier selection, etc., can be assessed.

In order to overcome the limitations of the previous mentioned approaches and with the aim of providing an integrated formulation, operations considerations are included in the model proposed in this work. Several decisions could be incorporated. However a detailed production program with MPC has been chosen taking into account that this decision determines the production rate that significantly affects other operational aspects as production flows, inventory levels, procurement and transport policy.

In this work, a MILP model for the simultaneous supply chain design and multiproduct plant design including detailed production planning is presented. This approach involves novel features in modeling detailed SC performance. The main challenge of modeling this problem arises from the incorporation of the detailed design and the production planning through MPC for each multiproduct semi-continuous/batch ethanol plant considered in the network. A priori, for these plants, the production of each product and their amounts are unknown.

The proposed model involves the integration of SC decision levels and represents a tool for providing decision support for different scenarios. Although a simplified ethanol production process has been considered, it will be shown through the examples that including detailed plant performance model has influence in the overall SC design. On the other hand, to the best of our knowledge, there are few works that integrates derivatives productions from process waste ([23,24]). In this work, yeasts production is performed in order to reduce ethanol process disposals. Therefore, additional stages are considered for each ethanol plant in order to evaporate and dry the process disposals. Thus, tradeoffs between design and environmental decisions, like unit sizes and residue recycles, are assessed. The capabilities of the presented formulation are illustrated through the examples, where different scenarios are evaluated and several tradeoffs are analyzed.

The remainder of this article is organized as follows. The problem statement and modeling assumptions are next described. The proposed mathematical model is presented in Section 3. In Section 4, five examples are illustrated and their results are analyzed. The conclusions of the work are finally drawn in the last section of the paper.

2. Problem statement

The SC considered in this work comprises three echelons: raw material sites, ethanol/yeast production facilities, and client zones. Near to each raw material site *s*, a maximum amount of sugar cane,

 QSC_s^{UP} , is available for producing sugar and molasses. In this work, sugar production and distribution is not modeled, but it can be easily incorporated to the formulation. Molasses can be distributed from raw material sites s ($s = 1, ..., N_s$) to plants f ($f = 1, ..., N_f$) to produce ethanol. Each installed plant can produce the three products: torula yeast, ethanol and baker's yeast, and they have the process stages as shown in Fig. 1. Then, the final products are transported from each facility to customer zones c ($c = 1, ..., N_c$) in order to fulfill their demands. The minimum and maximum demands of each product at each customer zone, DM_{ic}^{LO} and DM_{ic}^{UP} , for i = torula yeast, ethanol and baker's yeast, are model parameters.

This work assumes a simplified production process taking into account that the main objective of this article is the appropriate assessment of the integrated management of the bioethanol production. Ethanol and baker's yeast are simultaneously produced. The stages involved in ethanol production process are batch biomass fermentation, two units in series for alcohol fermentation, semicontinuous centrifugation and distillation. Baker's yeast can be produced simultaneously with ethanol production evaporating and drying of the centrifugation residue of this process. That means that when the ethanol fermented broth is centrifuged, the solids can be evaporated and dried in order to produce baker's yeast while the liquids are distilled for producing ethanol.

Torula yeast is produced through batch biomass fermentation, and a semicontinuous train given by centrifugation, evaporation and drying stages. This yeast is used for cattle feed.

The distillation is composed by two batch items: the distiller feed vessel and the distillate tank, and three semicontinuous items: the evaporator, the condenser and the column itself. The model determines the number of parallel units for each batch stage, while for semicontinuous stages only one unit per stage is used.

This class of plants is namely "sequential multipurpose batch plants" [25], and from the mathematical modeling standpoint presents a big challenge. For designing the plants, the number of out of phase parallel units for each batch stage must be determined as well as the sizing for batch and semicontinuous units. For the design, the units for distillation stage are treated as individual stages. But when the distillation stage is duplicated, all the distillation items are duplicated taking identical sizes. However, for production scheduling, the considered stages for ethanol/baker's yeast productions are five since in the semicontinuous subtrain all the stages (centrifugation, evaporation and drying) have the same processing time, and distillation processing time is unique for all the items involved in this stage. For torula production, two stages are considered for the scheduling: biomass fermentation and the semicontinuous subtrain.

Molasses are fed to biomass fermentors of ethanol production, while torula biomass fermentors are fed with an ethanol distilled residue called vinasses. Due to vinasses degradation, a continuous supply of this residue must be assured. Therefore, MPC is the most convenient scheduling policy for planning these productions, in order to fulfill the demands in the time horizon of each installed plant H_f . Moreover, a maximum number of batches of each product in the campaign, NBC_{if}^{UP} , is allowed, and the number of campaign repetitions, NN_f , is discretized considering the minimum and maximum number of times that the production campaign of each plant can be cyclically repeated along the planning horizon, NN_f^{LO} and NN_f^{UP} respectively.

Therefore, the problem goal consists of jointly determining:

(a) The design of the SC: (i) production plants location; (ii) molasses supply from each sugar cane plant; (iii) ethanol and yeasts production in each installed plant; and, (iv) raw material and product flows among SC nodes.

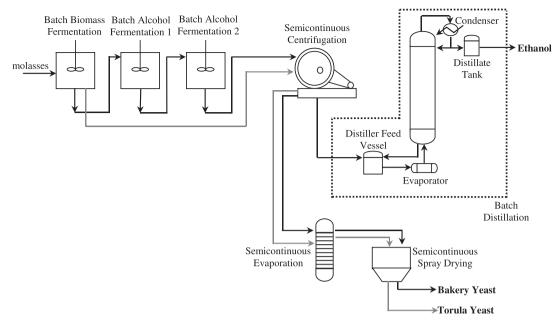


Fig. 1. Ethanol plant flowsheet.

- (b) The design of each installed plants: (i) plant configuration (the number of out of phase parallel units for batch stages);(ii) the unit sizes; and, (iii) the number and size of the product batches in each ethanol plant.
- (c) The detailed production planning for each installed ethanol/ yeast plant: (i) the campaign composition (number of batches for ethanol and yeast products in a campaign); (ii) batch assignment to units in each stage; (iii) sequence of batches on each unit; (iv) initial and final times for the batches in the campaign for each processing unit; and (v) the number of times that campaigns are repeated over the time horizon of each plant.

The performance measure is maximizing the net profit calculated as the benefits by sales minus the total annual cost, given by plants installation, investment, production, and transportation costs.

Unlike the previous work of Corsano et al. [23], this work incorporates production planning decisions through MPC and considers a MILP model instead of a MINLP one, by using a fixed size factor and time formulation. On the other hand, compared with the work of Fumero et al. [24], this work integrates SC optimization decisions to the model of ethanol plant design and production planning.

3. Model formulation

In this section the model for the simultaneous SC and facilities design including scheduling for ethanol and derivatives plants is presented.

3.1. SC design constraints

Let ex_f be the binary variable for plant allocation:

$$ex_f = \begin{cases} 1 & \text{if plant } f \text{ is installed,} \\ 0 & \text{otherwise} \end{cases}$$

Baker's yeast is a by-product of ethanol and they are simultaneously produced. However, sometimes baker's yeast should be not produced, for example when it is not profitable, and the centrifuged broth is discarded. As was previously mentioned, it is assumed that torula yeast is produced using distillery vinasses of ethanol process, and, if torula is not produced, vinasses are discarded. Therefore, torula yeast production is bounded according to the produced amount of ethanol, $Q_{et,f}$. The details of the considered technology, including mass balance coefficients, are shown in Fig. 2, and satisfy the following relations:

$$Q_{i,f} \le \rho_i Q_{et,f} \quad \forall i = \text{tor}, \text{bak}; \forall f$$
 (1)

where ρ_{tor} is a conversion factor calculated according to the produced vinasses from ethanol production (Mele et al. [17]) and ρ_{bak} is taken from Corsano et al. [26].

Plants are designed using a set of discrete unit sizes and the number of duplicated units is upper bounded, so installed plants have limited capacity. On the other hand, each raw material site s can produce a limited amount of molasses given by the available amount of sugar cane near each site:

$$QM_s \le \sigma_{mol}QSC_s^{UP} \quad \forall s \tag{2}$$

where QM_s represent the amount of molasses produced at site s and σ_{mol} the sugar cane-molasses conversion factor.

Molasses transportation from raw material sites to plants is given by the following constraints:

$$QM_s = \sum_f QR_{sf} \quad \forall s \tag{3}$$

$$QR_{sf} \le ex_f QM_s \quad \forall s, f \tag{4}$$

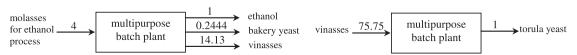


Fig. 2. Schematic representation of the adopted technology.

where QR_{sf} is the amount of molasses transported from s to f. Eq. (4) assures that if plant f is not allocated, QR_{sf} has to be zero, otherwise, the constraint results redundant.

Let fc_f be a conversion factor that indicates the kilograms of molasses per liter of ethanol ($fc_f = 0.25$ according to Fig. 2). Then,

$$\sum_{i} QR_{sf} = fc_f Q_{if} \quad \forall f, i = \text{et}$$
 (5)

expresses the amount of molasses needed to produce ethanol in plant f.

For the mass balances between production plants and customer zones, the continuous variable QC_{ifc} is defined as the amount of product i delivered from plant f to customer zone c. In this case, the final products are three: ethanol, baker's yeast and torula yeast. Then, assuming that the total amount of product i manufactured at plant f is delivered to customer zones (no product storage in plant), the following constraint is posed:

$$\sum_{i} QC_{ifc} = Q_{if} \quad \forall i, f$$
 (6)

It worth to be noted that if plant f is not installed, that is $ex_f = 0$, then the amount of i delivered from this plant to each customer zone c has to be zero. Otherwise, the total amount of i delivered from plant f to customer zone c has to be at least the minimum demand or at most the maximum demand of that product in that customer zone:

$$ex_f DM_{ic}^{LO} \le QC_{ifc} \le ex_f DM_{ic}^{UP} \quad \forall i, f, c$$
 (7)

Finally, the demand of each product in each customer zone has to be fulfilled:

$$\sum_{f} QC_{ifc} \leq DM_{ic}^{UP} \quad \forall i, c$$
 (8)

$$\sum_{f} QC_{ifc} \ge DM_{ic}^{LO} \quad \forall i, c$$
 (9)

3.2. Plant design constraints

In this section, the plant design restrictions are formulated. This part of the model is largely inspired in the formulation presented by Fumero et al. [24]. In this approach some modifications were introduced in order to embed the previous formulation into the overall SC model. Basically, several constraints were reformulated due to production targets in each plant are optimization variables, whereas in [24] these were known parameters. Therefore, they are presented in order to make comprehension of the model easier.

Given that products can follow a different production path, the sets ES_i and EB_i are introduced to represent the semicontinuous and batch processing stages, respectively, used to manufacture product i. Specifically, in this work the considered sets are: $EB_{tor} = \{\text{biomass fermentor}\}$, $ES_{tor} = \{\text{centrifugation, evaporator and dryer}\}$, $EB_{et} = \{\text{biomass fermentor, ethanol fermentor 1, ethanol fermentor 2, distillation}\}$, $EB_{et} = \{\text{centrifugation}\}$, $ES_{bak} = \{\text{centrifugation, evaporator and dryer}\}$.

As was previously mentioned, units duplication is allowed for batch stages. Therefore, a new decision variable is introduced to determine the number of allocated units to each batch stage. Let z_{ikf} be the binary variable for unit assignment:

$$z_{jkj} = \begin{cases} 1 & \text{if unit } k \text{ of stage } j \text{ of plant } f \text{ is employed,} \\ 0 & \text{otherwise} \end{cases}$$

In order to reduce the search space and without loss of generality, it is assumed that available units for each batch stage are utilized in ascending order. The following expression establishes that unit k+1 is only allocated if unit k has been already used:

$$z_{jkf} \ge z_{jk+1,f} \quad \forall j \in EB_i, 1 \le k \le K_{jf} - 1, f$$

$$\tag{10}$$

where K_{jf} correspond to the maximum number of parallel units that can be allocated in stage j. Taking into account that binary variable z_{jkf} establishes if unit k is allocated in batch stage j of plant f, then, summing on k it is possible to determine the total number of units operating in stage j.

For sizing the units of each stage j of each plant f, V_{jf} , the following equation is stated (Biegler et al. [27]):

$$V_{if} \ge SF_{ii}B_{if} \quad \forall i, j \in EB_i, f \tag{11}$$

where B_{ij} is the batch size and SF_{ij} is the size factor which represents the required size in stage j to produce a unit of mass of final product i [27]. The right-hand side determines the minimum capacity required at stage j for production of product i. Thus, Eq. (11) assures that the unit sizes of stage j in plant j allow to process all products.

For semicontinuous stage j, the unit dimension is given by a processing rate, R_{jj} . It is calculated using the duty factor, D_{ij} , which is defined as a constant equivalent to the size factor, the processing time, t_{ij} , and the batch size, B_{ij} , for every product i processed at this stage:

$$R_{jf} \ge \frac{D_{ij}}{t_{ij}} B_{if} \quad \forall i, j \in ES_i, f$$
 (12)

In this work, it is assumed that all the possible installed plants have the same technology, and then the processing times as well as the duty and size factors are identical for all of them.

The total number of batches of product i in each plant over the time horizon H_f , symbolized by NB_{if} , depends on the product demand Q_{if} and the batch size B_{if} , and is defined by:

$$NB_{if} = \frac{Q_{if}}{B_{if}} \quad \forall i, f \tag{13}$$

The decision variables NC_f and NBC_{if} are introduced to represent the number of times that the MPC will be cyclically repeated over the horizon H_f and the number of batches of each product i that take part in the campaign, respectively. Then, the following equation represents the relation among these variables:

$$NBC_{if}NC_f = NB_{if} \quad \forall i, f$$
 (14)

The following expressions are obtained by substituting Eqs. (13) and (14) into Eqs. (11) and (12):

$$V_{jf} \ge \frac{SF_{ij}Q_{if}}{NBC_{if}NC_{f}} \quad \forall i, j \in EB_{i}, f$$
 (15)

$$R_{jf} \ge \frac{D_{ij}Q_{if}}{t_{ij}NBC_{if}NC_{f}} \quad \forall i, j \in ES_{i}, f$$

$$(16)$$

In order to determine the number of batches of product i that composes the MPC, a new binary variable is introduced:

$$x_{inf} = \begin{cases} 1 & \text{if } n \text{ batches of product } i \text{ are processed} \\ & \text{in the campaign of plant } f \\ 0 & \text{otherwise} \end{cases}$$

In order to ensure that exactly one option is selected, the following expression is posed:

$$\sum_{n=1}^{NBC_{i}^{UP}} x_{inf} = ex_{f} \quad \forall i, f$$
 (17)

Therefore,

$$\sum_{n=1}^{NBC_{if}^{UP}} n \quad x_{inf} = NBC_{if} \quad \forall i, f$$
 (18)

The unit sizes V_{jf} and R_{jf} are available in discrete sizes, $SV_{jf} = \{VF_{j1f}, VF_{j2f}, \dots, VF_{jP_{jf}f}\}$ and $SR_{jf} = \{RF_{j1f}, RF_{j2f}, \dots, RF_{jM_{jf}f}\}$ respectively, which correspond to the available commercial dimensions for this equipment. Then, the following binary variable is defined for selecting a discrete value for each unit size:

$$v_{jpf} = \begin{cases} 1 & \text{if units of batch stage } j \text{ have size } p \text{ in plant } f \\ 0 & \text{otherwise} \end{cases}$$

$$r_{jmf} = \begin{cases} 1 & \text{if units of semicontinuous stage } j \text{ have size } m \text{ in plant } f \\ 0 & \text{otherwise} \end{cases}$$

Then, the dimension of equipment in batch stage j for each installed plant is given by:

$$V_{jf} = \sum_{p} \nu_{jpf} V F_{jpf} \quad \forall j \in \bigcup_{i} EB_{i}, f$$
 (19)

whereas in semicontinuous stage j is given by:

$$R_{jf} = \sum_{m} r_{jmf} RF_{jmf} \quad \forall j \in \bigcup_{i} ES_{i}, f$$
 (20)

where

$$\sum_{p} \nu_{jpf} = ex_f \quad \forall j \in \bigcup_{i} EB_i, f$$
 (21)

and

$$\sum_{m} r_{jmf} = ex_f \quad \forall j \in \bigcup_{i} ES_i, f$$
 (22)

Then, substituting Eqs. (18)–(20) into Eqs. (15) and (16), the following expressions are obtained:

$$NC_f \ge \sum_{p} \sum_{n=1}^{NBC_i^{UP}} \frac{SF_{ij}Q_{if}}{VF_{jpf}n} v_{jpf} x_{inf} \quad \forall i, j \in EB_i, f$$
 (23)

$$NC_{f} \geq \sum_{m} \sum_{n=1}^{NBC_{i}^{UP}} \frac{D_{ij}Q_{if}}{t_{ij}RF_{jmf}n} r_{jmf} x_{inf} \quad \forall i, j \in ES_{i}, f$$
 (24)

The nonlinear factors $Q_{if}v_{ipf}v_{inf}$ and $Q_{if}r_{jmf}v_{inf}$ in Eqs. (23) and (24) are eliminated by introducing the following decision variables:

$$w_{ijpnf} = \begin{cases} Q_{if} & \text{if both } v_{jmf} \text{ and } x_{inf} \text{ are } 1 \\ 0 & \text{otherwise} \end{cases}$$

$$u_{\mathit{ijmnf}} = \left\{ egin{array}{ll} Q_{\mathit{if}} & \mathrm{if~both~} r_{\mathit{jmf}} \ \mathrm{and~} x_{\mathit{inf}} \ \mathrm{are~} 1 \\ 0 & \mathrm{otherwise} \end{array}
ight.$$

and the following constraints must be hold:

$$\sum_{p} w_{ijpnf} \leq Q_{if}^{UP} x_{inf} \quad \forall i, j, f, n$$
 (25)

$$\sum_{n} w_{ijpnf} \leq Q_{if}^{UP} v_{jpf} \quad \forall i, j, f, p$$
 (26)

$$\sum_{n}\sum_{p}W_{ijpnf}=Q_{if}\quad\forall i,j,f \tag{27}$$

$$\sum_{i} u_{ijmnf} \leq Q_{if}^{UP} x_{inf} \quad \forall i, j, f, n$$
 (28)

$$\sum_{n} u_{ijmnf} \leq Q_{if}^{UP} r_{jmf} \quad \forall i, j, f, m$$
 (29)

$$\sum\sum u_{ijmnf} = Q_{if} \quad \forall i, j, f \tag{30}$$

Therefore, Eqs. (25) and (24) can be expressed using linear inequalities:

$$NC_f \ge \sum_{n} \sum_{n=1}^{NBC_{ij}^{UP}} \frac{SF_{ij}}{VF_{jpf}n} w_{ijpnf} \quad \forall i, j \in EB_i, f$$
 (31)

$$NC_f \ge \sum_{m} \sum_{n=1}^{NBC_{ij}^{UP}} \frac{D_{ij}}{t_{ij}RF_{jmf}n} u_{ijmnf} \quad \forall i, j \in ES_i, f$$
 (32)

For each installed plant, the MPC is cyclically repeated over H_f . Therefore, the MPC cycle time, CTC_f , multiplied by the number of times that the campaign is repeated, NC_f , cannot exceed the time horizon H_f :

$$CTC_fNC_f \le H_f \quad \forall f$$
 (33)

Then, in order to avoid nonlinearity of Eq. (33), the variable NC_f is uniformly discretized in the interval $[NC_f^{LO}, NC_f^{UP}]$ through N_f points appropriately suggested, called tt_{df} , $d = 1, ..., N_f$. Thus, the following binary variable is defined:

$$\mathit{NNC}_\mathit{df} = \begin{cases} 1 & \text{if the campaign is repeated} \ \ \mathit{tt}_\mathit{df} \ \ \mathsf{times in plant} \ f, \\ 0 & \text{otherwise} \end{cases}$$

The following expression is introduced to represent the number of times that the MPC is cyclically repeated over H_f in plant f:

$$NC_f = \sum_{d=1}^{N_f} tt_{df} NNC_{df} \quad \forall f$$
 (34)

with:

$$\sum_{d=1}^{N_f} NNC_{df} = ex_f \quad \forall f \tag{35}$$

Then, substituting Eq. (34) into Eq. (33), the following constraints must be satisfied:

$$CTC_{f} \sum_{d=1}^{N_{f}} tt_{df} NNC_{df} \le H_{f} \quad \forall f$$
(36)

Or equivalently:

$$\sum_{d=1}^{N_f} tt_{df} NNC_{df} CTC_f \le H_f \quad \forall f$$
 (37)

New nonnegative continuous variables ww_{df} are introduced to represent the bilinear terms NNC_{df} CTC_f in order to avoid the nonlinearities in Eqs. (37). Substituting the bilinear terms with this new variable, the following expression is obtained:

$$\sum_{d=1}^{N_f} tt_{df} ww_{df} \le H_f \quad \forall f$$
 (38)

where the following constraints must be also considered:

$$\sum_{d} ww_{df} = CTC_f \quad \forall f \tag{39}$$

$$ww_{df} \leq CTC_f^{UP}NNC_{df} \quad \forall d, f$$
 (40)

where CTC_f^{UP} corresponds to an upper bound for the variable CTC.

3.3. Scheduling constraints

For modeling the batch assignment to each unit in each plant, an asynchronous slot-based continuous-time formulation is adopted. A slot is a time interval of variable length where a batch will be assigned. The basic ideas of this scheduling representation

are taken from Fumero et al. [28]. According to that work, the following expression is posed to specify the tighter maximum number of slots postulated for unit k of stage j of plant f, L_{kif} .

$$L_{kjf} = \left| \frac{\sum_{i \in I_j} NBC_{if}^{UP}}{k} \right|, \quad \forall j, 1 \le k \le K_{jf}, f$$

$$(41)$$

where I_j represents the set of products that stage j can process. As was previously mentioned, all installed plants have the same technology, and, then, the sets I_j are the same for all plants. Therefore, in a campaign, the maximum number of batches of product i is NBC_{if}^{UP} , and, the maximum number of batches that can be processed in stage j is $\sum_{i \in I_i} NBC_{if}^{UP}$.

A new binary variable is included in order to represent the assignment of batches to specific slots of units in each stage of a plant *f*:

$$Y_{bjklf} = \begin{cases} 1 & \text{if batch } b \text{ is assigned to slot } l \text{ and processed} \\ & \text{in unit } k \text{ of stage } j \text{ of plant } f \\ 0 & \text{otherwise} \end{cases}$$

If plant f is installed, each batch of product i in the campaign processed at stage j, is at most assigned to a slot of a unit of this stage:

$$\sum_{\substack{1 \\ 1 \le l \le l_{kif}}} \sum_{\substack{1 \\ 1 \le k \le K_{if}}} Y_{bjklf} \le ex_f \quad \forall j, i \in I_j, b \in BI_{if}, f$$

$$\tag{42}$$

On the other hand, each slot l of unit k at stage j is only employed for processing at most one batch if plant f is installed. Then, the following inequality must be added:

$$\sum_{b \in \cup_{i \in I_{if}} Bl_{if}} Y_{bjklf} \le ex_f \quad \forall j, 1 \le k \le K_{jf}, 1 \le l \le L_{kjf}, f \tag{43}$$

It is worth mentioning that in each slot l of a specific unit k at most one batch i can be processed. If no product is assigned to slot l, its length will be zero, and therefore, initial and final times of that slot are equal and coincide with the final time of the previous slot. Then, taking into account that the number of slots proposed in each unit is overestimated, some of them may be empty.

The following constraint ensures that for each product *i* the set of batches to be processed in the stages that form part of the production path of this product should be the same:

$$\sum_{\substack{1 \\ 1 \le l \le l_{kff} 1 \le k \le K_{lf}}} \sum_{\substack{k \\ 1 \le k \le K_{lf}}} Y_{bjklf} = \sum_{\substack{1 \\ 1 \le l \le l_{kff} 1 \le k \le K_{ff}}} \sum_{\substack{k \\ k \le K_{ff}}} Y_{bj'klf} \quad \forall j,j',j < j',b \in \cup_{\substack{i \\ i \in (l_j \cap l_{f'})}} B I_{if},f$$
 (44)

Eq. (45) reduces the number of alternative solutions, adding the batches of a same product in the campaign in ascending order.

$$\sum_{1 \le k \le K_{ff}} \sum_{1 \le l \le k_{kf}} Y_{bjklf} \ge \sum_{1 \le k \le K_{ff}} \sum_{1 \le l \le k_{kf}} Y_{b+1jklf} \ \forall j, i \in I_{j}, b \in BI_{if}, b+1 \in BI_{if}$$
 (45)

Finally, the total number of batches of product i composing the campaign in a plant f, NBC_{if} , is defined using variable Y_{bjklf} :

$$NBC_{if} = \sum_{b \in Bl_{if}} \sum_{1 \le k \le K_{if}} \sum_{1 \le l \le L_{kif}} Y_{bjklf} \quad \forall j, i \in I_j, f$$

$$(46)$$

With the objective of improving the computational performance, auxiliary variables and additional constraints are incorporated to the formulation. Also, the model considers several logical constraints between binary variables. For further details see Fumero et al. [28].

3.3.1. Timing constraints

A batch unit is characterized by filling, processing and emptying times, and possibly also a waiting time (idle time). Then, for each batch stage j involved in the production sequence of product i, the filling and emptying times may be considered as part of the time needed to process a batch of product i in stage j, depending on whether contiguous semicontinuous units exist or not. If a batch stage is preceded by a semicontinuous stage, then the processing time of the semicontinuous stage represents a "filling time" for the batch unit. On the other hand, if a batch stage is followed by semicontinuous stage, the processing time of the semicontinuous unit represents a "emptying time" for the batch unit.

Let T_{ij} be the processing time for product i in stage j. In this work it is assumed that all the plants have the same processing time for each stage. For ethanol/baker's yeast production the processes sequence is biomass fermentor, alcohol fermentors 1 and 2, centrifugation (evaporation and drying), and distillation. Centrifugation, evaporation and drying constitute a semicontinuous subtrain between two batch stages (alcohol fermentation 2 and distillation). Therefore, the time that a unit of alcohol fermentation 2 stage will be occupied ($T_{et,afer2}$) to process a batch of product i, is given by its processing time plus the processing time of semicontinuous subtrain, which represent an "emptying time". In the same way, the time that distillation units will be occupied considers a "filling time" equal to the semicontinuous subtrain processing time.

For torula yeast production, the stages sequence is biomass fermentation, centrifugation, evaporation, and drying. Therefore, the biomass fermentation units will be occupied during the emptying time to the semicontinuous subtrain, i.e. the centrifugation processing time. It is worth to mention that the processing times for units in the semicontinuous subtrain are equal. Since the material of both productions processed in the shared stages is similar, cleaning times can be assumed negligible or included in the processing time, and therefore, they are not considered in the current formulation.

Let Tl_{jklf} and TF_{jklf} be the initial and final times, respectively, of slot l in unit k of stage j of plant f. Thus, the relation between variables Tl_{jklf} , TF_{jklf} and Y_{bjklf} is established by the following equation:

$$TF_{jklf} = TI_{jklf} + \sum_{i} \sum_{b \in Bl_{if}} T_{ij} Y_{bjklf} \quad \forall j, 1 \le k \le K_{jf}, 1 \le l \le L_{kjf}, f$$
 (47)

Considering that a slot must not be necessarily used, when no batch occupies slot l in unit k of stage j of plant f (i.e. $Y_{bjklf} = 0$, $\forall b \in \bigcup_{i \in I_{if}} BI_{if}$), the initial and final times of this slot are equal, i.e. $TI_{jklf} = TF_{jklf}$.

The following constraint is added to avoid the overlapping among the processing times of different slots in a unit:

$$TF_{jklf} \le TI_{jkl+1f} \quad \forall j, 1 \le k \le K_{jf}, 1 \le l < L_{kjf}, f$$

$$\tag{48}$$

Besides, if no batch is assigned to slot l+1 of unit k at stage j of plant $f(\sum_{b\in Bl_{ij}} Y_{bjk,l+1,f} = 0)$, then the initial time of this slot is enforced to be equal to the finishing time of slot l. Then, taking into account that Eq. (48) is satisfied for successive slots in a unit, this new condition is represented by:

$$TF_{jklf} - TI_{jk,l+1,f} \ge -M_1 \sum_{b \in Bl_{if}} Y_{bjk,l+1,f} \quad \forall j, \ 1 \le k \le K_{jf}, 1 \le l < L_{kjf}, f$$
 (49)

where M_1 is a sufficiently large number that makes the constraint redundant when a product is assigned to slot l + 1.

3.3.2. Zero-wait (ZW) transfer policy

The ZW transfer policy assumes that a batch, after finishing its processing at a stage, must be transferred immediately to the next processing stage. Similar to equations of the previous sub-section, as the production path for each product is known, the equations for ZW policy are specifically stated.

For ethanol/baker's yeast production, the following equations must be satisfied:

ZW between biomass fermentation (bfer) and alcohol fermentation 1 (afer1) stages:

$$TF_{bfer,klf} = TI_{afer1,k'\ l'f} \ 1 \le k \le K_{bfer,f}, \ 1 \le k' \le K_{afer1,f},$$

$$k/Y_{b,bfer,klf} = 1, k'/Y_{b,afer1,k'l'f} = 1, b \in BI_{et,f},$$

$$1 \le l \le L_{k,bfer,f}, \ 1 \le l' \le L_{k'\ afer1,f},$$
(50)

ZW between alcohol fermentation 1(afer1) and alcohol fermentation 2 (afer2) stages:

$$TF_{afer1,klf} = TI_{afer2,k'l'f} \ 1 \le k \le K_{afer1,f}, 1 \le k' \le K_{afer2,f},$$

$$k/Y_{b,afer1,klf} = 1, k'/Y_{b,afer2,k'l'f} = 1, b \in BI_{et,f},$$

$$1 \le l \le L_{k,afer1,f}, 1 \le l' \le L_{k',afer2,f}, f$$
(51)

ZW between alcohol fermentation 2(afer2) and semicontinuous subtrain (cen) stages:

$$TF_{afer2,klf} = TI_{cen,k'l'f} \ 1 \le k \le K_{afer2,f}, \ 1 \le k' \le K_{cen,f},$$

$$k/Y_{b,afer2,klf} = 1, k'/Y_{b,cen,k'l'f} = 1, b \in BI_{et,f},$$

$$1 \le l \le L_{k,afer2,f}, \ 1 \le l' \le L_{k',cen,f}, f$$
(52)

ZW between semicontinuous subtrain (cen) and distillation (dis) stages:

$$TF_{cen,klf} = TI_{dis,k'\ l'f}\ 1 \le k \le K_{cen,f}, 1 \le k' \le K_{dis,f}, \\ k/Y_{b,cen,klf} = 1, k'/Y_{b,dis,k'l'f} = 1, b \in BI_{et,f}, \\ 1 \le l \le L_{k,cen,f}, \quad 1 \le l' \le L_{k',dis,f}, f$$
 (53)

Taking into account these constraints must be only satisfied when a batch is assigned to those slots and units, constraints of Big-M type are used:

$$\begin{split} TF_{\mathit{bfer,klf}} - TI_{\mathit{afer1,k'l'f}} &\geq M_2(Y_{\mathit{b,bfer,klf}} + Y_{\mathit{b,afer1,k'l'f}} - 2) \\ & 1 \leq k \leq K_{\mathit{bfer,f}}, 1 \leq k' \leq K_{\mathit{afer1,f}}, b \in \mathit{BI}_{\mathit{et,f}}, \\ & 1 \leq l \leq L_{\mathit{k,bfer,f}}, 1 \leq l' \leq L_{\mathit{k',afer1,f}}, f \end{split} \tag{54a}$$

$$\begin{split} -TF_{\textit{bfer,klf}} + TI_{\textit{afer1,k'l'f}} &\geq M_2(Y_{\textit{b,bfer,klf}} + Y_{\textit{b,afer1,k'l'f}} - 2) \\ 1 &\leq k \leq K_{\textit{bfer,f}}, 1 \leq k' \leq K_{\textit{afer1,f}}, b \in BI_{\textit{et,f}}, \\ 1 &\leq l \leq L_{\textit{k,bfer,f}}, 1 \leq l' \leq L_{\textit{k',afer1,f}}, f \end{split} \tag{54b}$$

where M_2 is a large number that relaxes these restrictions when batch b is not processed in slot l of unit k at stage bfer or in slot l' of unit k' at stage afer1.

Analogously to (54a) and (54b), the Big-M constraints are formulated for Eqs. (51)–(53).

Similarly to ethanol production, the ZW equations are stated for biomass fermentation and semicontinuous subtrain of torula production.

3.3.3. Cycle time of the campaign

For each installed plant f, the cycle time of the campaign, CTC_f is determined taking into account the number of times that the campaign is repeated over the time horizon. CTC_f is defined as the maximum difference between the final and initial operating times of the last slot and first slot assigned to each unit used in that plant:

$$CTC_f \ge TF_{jkL_{irf}} - TI_{jkl_{if}} \quad \forall j, 1 \le k \le K_{if}, f$$
 (55)

3.4. Objective function

The objective function is the maximization of the annual net benefit (*ANB*) given by the income for sales minus the total annual cost which considers installation cost, investment cost and transportation cost, described as follows.

3.4.1. Income for sales

$$IS = \sum_{f} \sum_{c} \sum_{i} pr_{i} QC_{ifc}$$
 (56)

where pr_i represents the selling price for product i.

3.4.2. Installation cost

$$INSC = \sum_{f} Inc_{f} ex_{f}$$
 (57)

where inc_f represents the installation cost for plant f.

3.4.3. Investment cost

The investment cost is given by the expression

$$INVC = CCF \sum_{f} \sum_{i} \sum_{k} \alpha_{jf} V_{jf}^{\beta_{jf}}$$
 (58)

where α_{jf} and β_{jf} are suitable cost coefficients for stage j, plant f. In order to take into account the amortization, a capital charge factor on the time horizon *CCF* is included.

Considering Eqs. (19) and (20), Eq. (58) can be re-written as:

$$INVC = CCF \sum_{f} \left(\sum_{\substack{j \in \bigcup_{EB_{if}} \sum_{k} \sum_{p} \alpha_{jf} VF_{jpf}^{\beta_{if}} z_{jkf} \ \nu_{jpf} + \sum_{\substack{j \in \bigcup_{ES_{if}} \sum_{k} \sum_{m} \alpha_{jf} RF_{jmf}^{\beta_{if}} z_{jkf} r_{jmf}}} \sum_{j \in \bigcup_{ES_{if}} \sum_{k} \sum_{j \in \bigcup_{ES_{if}} \sum_{ES_{if}} \sum_{j \in \bigcup_{ES_{if}} \sum_{ES_{if}} \sum_$$

The first term corresponds to batch units cost whereas the second one to semicontinuous units cost for each installed plant *f*.

Binary variables e_{jkpf} and ee_{jkmf} are introduced in Eq. (59) in order to eliminate nonlinearities. Variable e_{jkpf} links decision variables v_{jpf} and z_{jkf} such that e_{jkpf} takes value 1 if both are 1 and 0 otherwise, whereas variable ee_{jkmf} links decision variables r_{jmf} and z_{jkf} such that ee_{jkmf} takes value 1 if both are 1 and 0 otherwise. In order to enforce these relationships, the following constraints are included:

$$e_{jkpf} \geq v_{jpf} + z_{jkf} - 1 \quad \forall j \in \underset{i}{\cup} EB_{if}, 1 \leq k \leq K_{jf}, 1 \leq p \leq P_{jf}, f$$
 (60)

$$ee_{jkmf} \ge r_{jmf} + z_{jkf} - 1 \quad \forall j \in \underset{i}{\cup} ES_{if}, 1 \le k \le K_{jf}, 1 \le m \le M_{jf}, f$$
 (61)

If the following upper and lower bounds are defined, these new variables do not require to be defined as binary:

$$0 \le e_{jkpf} \le 1 \quad \forall j \in \bigcup_{i} EB_{if}, 1 \le k \le K_{jf}, 1 \le p \le P_{jf}, f$$
 (62)

$$0 \le ee_{jkmf} \le 1 \quad \forall j \in \bigcup ES_{if}, 1 \le k \le K_{jf}, 1 \le m \le M_{jf}, f$$
 (63)

Finally, the following lineal objective function can be defined:

$$INVC = CCF \sum_{f} \left(\sum_{\substack{j \in \bigcup_{EB_{if}} \\ i}} \sum_{\substack{k \\ p}} \sum_{\substack{p}} \alpha_{jf} VF_{jpf}^{\beta_{jf}} e_{jkpf} + \sum_{\substack{j \in \bigcup_{ES_{if}} \\ i}} \sum_{\substack{k \\ m}} \sum_{\substack{m}} \alpha_{jf} RF_{jmf}^{\beta_{jf}} e e_{jkmf} \right)$$

$$(64)$$

3.4.4. Transportation cost

The model considers raw material and product transportation costs

$$TRANC = Cfuel\left(\sum_{s,f} \frac{2dist1_{sf}}{5} \frac{QR_{sf}}{Cap_1} + \sum_{i,f,c} \frac{dist2_{fc}}{5} \frac{QC_{ifc}}{Cap_i}\right)$$
(65)

Thus, the first term considers molasses transportation cost from raw material site s to production plant f, where the first fractional factor is the fuel usage, determined from the total distance traveled in a trip ($2 \ dist1_{sf}$), the fuel consumption for transport ($5 \ L \ km^{-1}$), and the total number of trips (QR_{sf}/Cap_1). Cap_1 represent the capacity of the molasses truck ($25 \ ton$). Similarly, the second term represent the transportation of final products, where $dist2_{fc}$ represent the distances between plants and customers, and Cap_i the truck capacity for transporting product i ($tor = 25 \ t$, $et = 20 \ t$, $bak = 25 \ t$).

3.4.5. Sugar cane cost

This cost encompasses cane cultivation, harvest, transportation, fertilization, and related field work, and it is expressed according to Eq. (2) by:

$$SCC = \sum_{s} CSCane_{s} \frac{1}{\sigma_{mol}} QM_{s}$$
 (66)

where CSCane_s represents the unit cost for processed sugar cane at site s.

3.4.6. Operative cost

The operative cost considers a cost per ton of produced product in each plant:

$$OC = \sum_{i,f} Oper_{if} Q_{if}$$
 (67)

where $Oper_{if}$ represents the unit cost for produced product i in plant f

Therefore, the following objective function is proposed:

$$ANB = IS - (INSC + INVC + TRANC + SCC + OC)$$
(68)

Disposal cost will be considered in some examples and it will be opportunely presented in the next section.

4. Results and discussions

The capabilities of the proposed approach is illustrated through a case study involving five raw material sites, three possible locations for production plants and five customer zones with ethanol demands. It is assumed that if yeasts are produced, they are delivered to near customer zones because of its degradation. Therefore, this example considers three extra customer zones near to the different production plants which demand only yeasts.

Tables 1 and 2 show the parameters for ethanol plants obtained from a detailed model (Corsano et al. [26]). For each plant, five discrete sizes are available for designing the equipment as reported

Table 3. The same table shows the unit cost parameters. In Table 4 the operative costs are depicted.

Table 5 expresses the distances between raw material sites and production plants, plant installation costs, and the availability of sugar cane at each site, while Table 6 shows the distances between plants and customer zones. c1–c5 represent clients with ethanol demand, while c6–c8 represent clients with yeast demand. In this last table, the maximum demands of ethanol are also given, while the maximum demands of torula and baker's yeasts are calculated using relation given by Eq. (1) and Fig. 2. For all products, the minimum demands are considered to be zero.

For production planning decisions, the maximum number of batches in the campaign of each installed plant is equal to 4 for ethanol and 3 for torula, while the number of campaign repetitions is discretized according to Eq. (34) considering 18 elements, where $NC_f^{LOW}-135$ and $NC_f^{UP}=315$. Therefore, the step size adopted is equal to 10, and the recurrence relation $tt_{df}=tt_{d-1f}+10$ for d=2, ..., 18 with $tt_{1f}=135$. The time horizon for each plant is equal to 7500 h/year.

The fuel cost, *Cfuel*, is assumed to be 2 \$/L, while product prices are 200 \$/t for torula and baker's yeast, and 860 \$/t for ethanol. Sugar cane cost is adopted equal to 4 \$/t and the sugar cane-molasses conversion factor, σ_{mol} , 0.0494. These data are representative and they are not actual prices, only ethanol price and σ_{mol} were adopted from [17].

Following, several scenarios are posed with the aim of analyzing suitable design for SC and production plants. Table 7 resumes the different studied cases and its characteristics. The model size of the different cases analyzed in this paper is large due to the several decisions which are simultaneously considered. Precisely, the presented approach has near 2200 binary variables, 5800 continuous variables and 17,100 constraints. All the models were implemented and solved in GAMS ([29]) in an Intel Core i7, 2.8 GHz processor. The time limit for solving the instances was 7200 CPU seconds (2 h) and the final optimality gap was always under 1%.

4.1. Case A

In this case, the approach is applied to the problem data previously presented; neither additional constraint nor parameters changes are considered.

The optimal solution allocates two production plants (f1 and f3) for producing ethanol and both yeasts. Molasses are transported from s1, s2 and s3 sites where sugar cane is processed. The maximum ethanol demand is supplied to customer c1–c5. Plant f1 produces 110,000 t/year of ethanol while f3 70,000 t/year, and both plants produce the maximum amount of baker's yeast according to Eq. (1), i.e. 26,884 t and 17,108 t respectively. However, produced vinasses are not totally used, since plant f1 discards 117,171 t of vinasses, and therefore, the maximum torula demand is not fulfilled for neighboring clients. Fig. 3 shows the SC design. If the total vinasses are recycled, bigger unit sizes are needed for evaporation and drying, and therefore the investment cost is

Table 1Size and duty factors for ethanol plant.

	Size and duty factors: SF_{ij} and D_{ij} (×10 ⁻²)										
	Fermentation		Semicontinuous subtrain I			Distillation					
	1	2	3	4	5	6	7	8	9	10	11
Torula yeast Ethanol/Baker's yeast	2.5 0.473	0 0.54	0 0.612	58.8 58.8	1.14 1.14	22 22	0 0.45	0 2.33	0 0.0972	0 3.94	0 0.127

Table 2 Processing times for stages of ethanol plant.

	Processing time: t_{ij} (h)	Processing time: t_{ij} (h)							
	Biomass fermentation	Alcohol fermentation 1	Alcohol fermentation 2	Semicontinuous subtrain	Distillation				
Torula yeast	10.74	0	0	5.22	0				
Ethanol/Baker's yeast	9.83	4.83	6.14	5.85	18.69				

 Table 3

 Available discrete sizes and cost coefficients for plant stages.

Units	Discrete un	it sizes: VF _{jp} and RI	Cost coefficient	Cost exponent			
	1	2	3	4	5	$lpha_j$	eta_j
1 (m ³)	150	350	550	700	1100	40,020	0.60
$2 (m^3)$	200	350	400	700	1400	24,200	0.45
$3 (m^3)$	235	470	800	940	1600	24,200	0.45
4 (kWh)	40	50	80	100	160	25,000	0.68
5 (m ²)	7	15	30	60	120	30,300	0.53
6 (m ²)	65	130	200	260	400	59,600	0.60
$7 (m^3)$	175	350	600	700	1200	31,100	0.60
$8 (m^2)$	75	150	300	600	900	9760	0.65
9 (m ²)	2	4	6	8	10	151,312	0.65
10 (m ²)	100	200	300	400	600	7255	0.65
11 (m ³)	50	100	150	200	300	31,100	0.60

References: 1: biomass fermentor, 2: alcohol fermentor 1, 3: alcohol fermentor 2, 4: centrifuge, 5: evaporator, 6: dryer, 7: distiller feed vessel, 8: distiller evaporator, 9: column, 10: condenser, 11: distillate tank.

 Table 4

 Operative costs for producing each product in each plant (\$/t).

	f1	f2	f3
Torula yeast	0.8	1	0.5
Ethanol	1.5	2.5	2.5
Baker's yeast	0.8	1.2	1

Table 5
Distances (km) between raw material sites and production plants, sugar cane availability (t/year), and plant installation costs (\$).

	f1	f1	f3	Sugar cane availability
s1	0	328	520	12,220,000
s2	352	0	220	4,324,000
s3	310	90	0	2,068,000
s4	1764	1092	850	125,960
s5	1086	1165	930	62,040
Installation costs	1,000,000	1,500,000	850,000	

increased. Therefore, a tradeoff between torula selling price and unit sizes (i.e. investment cost) is held.

The configuration of both production plants are similar, but with different unit sizes. Fig. 4 depicts the plant designs. The production campaign are also similar for both plants: the campaign is composed by two batches of ethanol and two batches of torula, the campaign cycle time is equal to 24.54 h and the campaign is 305

times repeated over the time horizon. First column of Table 8 shows the economical results for this case.

In order to compare the proposed approach with hierarchical methods, this example is solved for designing the SC first and then, the design and production planning of the involved plants are obtained. The sequential approach involves two steps: in the first, the SC design is solved, where the model formulation involves Eqs. (1)-(9) with the objective of maximizing the net annual profit without considering the investment cost. The optimal solution of this step allows obtaining the network configuration (plants number and localization), the flows among SC nodes, and production of each installed plant. In the second step, taking into account production targets i.e. fixing variable Qif, the problem is focused on determining the design and the optimal production campaign for each plant selected in the first stage, considering in the objective function the investment cost. When the SC design is solved, the optimal solution selects plant f1 and f3. Plant f1 produces 151,039 t/year of ethanol, 36,914 t/year of baker's yeast and 28,193 t/year of torula, while f3 produces 28,961 t/year of ethanol, 7078 t/year of baker's yeast, and 5406 t/year of torula. These production targets are fixed and the second stage is solved. But, the problem for the second stage is infeasible, since it is impossible to accommodate the fixed production targets of plant f1 in the available discrete unit sizes in the given time horizon. For obtaining a feasible (and optimal) solution, the discrete unit sizes must to be bigger than those proposed in Table 3, or the time horizon must be longer than 7500 h in order to produce more batches of each product. This is a disadvantage of sequential methods where production targets are optimized without taken into account design and production planning variables, while in the proposed simulta-

Table 6Distances (km) between plants and customer zones, and maximum product demands.

	c1	c2	c3	c4	c5	c6	c7	c8
f1	1229	1286	319	764	2728	10	1000	1000
f2	1565	822	500	1092	3014	1000	10	1000
f3	542	1599	45	1077	2990	1000	1000	10
Max. ethanol demand (t/year)	20,000	30,000	50,000	40,000	40,000	0	0	0

Table 7Characteristics of different studied cases.

	Yeast selling price (\$/t)	Allows residue disposals	Penalizes disposals
Case A	200	No	No
Case B	200	No	No
Case C	50	Yes	No
Case D	50	Yes	Yes

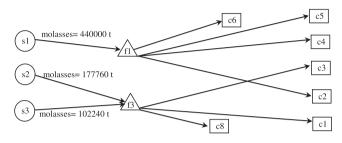


Fig. 3. SC optimal design for Case A.

neous approach evaluates jointly the tradeoffs among costs (involved in SC design and plant design and operation), production, unit sizes and number and size of batches to be produced in each plant. Even when a feasible solution is reached, the optimal solution obtained by sequential approach can be equal or worse than the one of simultaneous approach. Since the set of feasible solutions of a sequential approach is included in the set of feasible solutions of a simultaneous approach, then the optimal solution obtained by a hierarchical approach will be never better than the optimal solution given by a simultaneous approach.

4.2. Case B

Because of pollution problems, the reuse and treatment of distillery wastewater, generally known as vinasses, is one of the most significant and challenging issues in the industrial production of ethanol in order to assure the sustainability of the process. Concentration–incineration of vinasses, which can provide a satisfactory solution to the pollution problem, is an alternative, but its expensiveness constitutes a drawback ([30]). In this study case, the reuse of the total produced vinasses and centrifuged broth is considered

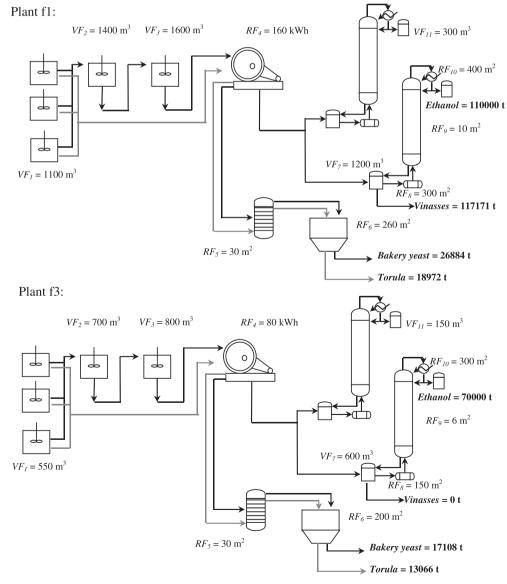


Fig. 4. Optimal plant designs for Case A.

with the aim of evaluating the production without ethanol wastes. This case forces to produce torula and baker's yeast using the total ethanol residues, i.e. centrifuged cream for baker's yeast and vinasses for torula yeast. Therefore, Eq. (1) must be satisfied with equality.

In this case, the optimal solution also selects plants f1 and f3, but the ethanol and yeasts amounts produced in each one are different to the values obtained in case A. Now, both plants are identical and their configuration and unit sizes are shown in Fig. 5, where SC design is also depicted. In the second column of Table 8 the economical results are shown. As can be noted the objective function for this case is only 0.5% worsen. Even though there are few differences between both optimal solutions, it is worth noting that plants of Case A are smaller than those of this studied case, and therefore it is not possible to reach the yeast production of Case B in the plants designed in Case A. Also it is not possible to produce more batches of torula in the time horizon to attain the yeast production of Case B with the plant design of case A, i.e. the campaign cycle time cannot be augmented, nor can more campaigns be added in the time horizon. Therefore, several elements

are simultaneously adjusted and ethanol production is arranged in a different manner in case B to satisfy the new requirements, although the total costs are increased. Again, in this studied case, the advantages of the simultaneous optimization are highlighted.

4.3. Case C

In this case it is assumed that torula and baker's yeast selling price is decrease to 50 \$/t, while all the remaining parameters stay as in case A. The optimal solution selects plants f1 and f3, with plant designs as shown Fig. 6, but in this case, the plant designs and production planning are very different from the previous cases. When torula selling price is reduced, torula production is also reduced. Ethanol remains profitable, so its maximum demand is produced. The production of baker's yeast results profitable, i.e. it is convenient to add the evaporator and dryer. However, torula production is not profitable considering its selling price and the semicontinuous subtrain investment cost. Therefore, torula is only produced in order to cover the idle times in semicontinuous subtrain of ethanol production. Two biomass fermentors are needed

Table 8Economical results for different studied cases (\$/year).

Sales and costs	Case A	Case B	Case C	Case D
Torula sales	6,407,600	6,719,800	809,800	1,605,500
Ethanol sales	154,800,000	154,800,000	154,800,000	154,800,000
Baker's yeast sales	8,798,400	8,798,400	2,199,600	2,199,600
IS	170,006,000	170,318,200	157,809,400	158,605,100
Molasses transportation	1,251,400	2,218,500	1,094,100	1,262,200
Torula transportation	10,252	10,751	5,182	10,275
Ethanol transportation	7,654,000	7,860,700	7,715,200	7,658,000
Baker's yeast transport.	14,077	14,077	14,077	14,077
INSC	1,850,000	1,850,000	1,850,000	1,850,000
INVC	9,292,700	8,896,100	8,183,300	9,292,700
SCC	58,252,000	58,252,000	58,252,000	58,252,000
Operative cost	400,326	421,159	383,708	400,769
Total costs	78,724,755	79,523,259	77,497,567	78,303,791
ANB	91,281,245	90,794,941	80,311,833	80,301,309

^a Including ResC = \$558,690.

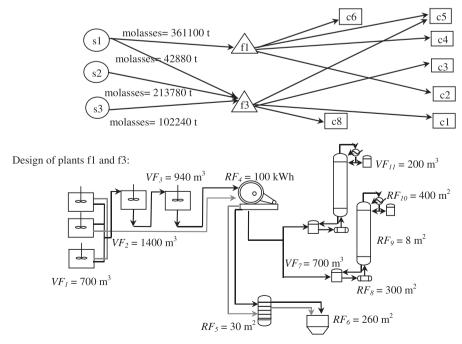


Fig. 5. SC and plants design for case B.

in order to preserve the campaign cycle time (if the campaign cycle time is augmented, the unit sizes must to be increased for producing the same amount of ethanol). In this way, the production campaign for both plants is composed by two batches of ethanol and one batch of torula as it is shown in Fig. 7.

Product distribution is also different from previous cases as can be noted in Fig. 8 where SC is shown. In the third column of Table 8 the economical results are stated and they are compared with previous cases, taking into account that only the selling price for both veasts is different from Case A and B: The income for sales is decreased because selling prices and produced torula are decreased. Molasses transportation cost is decreased since plant f1 produces a bigger amount of ethanol and this plant is next to raw material site s1 which is the major molasses producer according to the available sugar cane. Investment cost is also reduced because both plants have one unit less than in previous cases. operative cost is also decreased because smaller amount of torula is produced, and the sugar cane cost is the same in all cases since the amount of total processed cane for producing molasses is the same because the maximum demand of ethanol is always attained. In summary, when the torula selling price is reduced this production is not profitable, less amount of torula is produced and larger amount of vinasses are discarded. From the economical point of view, the income for sales is reduced but the transportation and investment costs are also decreased.

4.4. Case D

According to Case C, when torula selling price is not attractive, vinasses are discarded. Now, a new scenario is posed where also

residue disposal is penalized. Therefore, a cost due to process residue is added to the objective function. This penalization considers the vinasses not used for torula production and the centrifuged cream not used for baker's yeast. Let $Vres_f$ be the discarded vinasses and $VCres_f$ the discarded centrifuged cream for plant f; then, according to the relation of Fig. 2:

$$Vres_f = 14.13Q_{etf} - 75.75Q_{tor,f} (69)$$

$$VCres_f = 0.22875Q_{et.f} - 0.9358Q_{bak.f}$$
 (70)

The first term of Eq. (69) represents the total produced vinasses at plant f, while the second term is the total vinasses used for torula production in that plant. Similarly, the first term of Eq. (70) describes the total available centrifuged cream for producing baker's yeast in ethanol process and the second one is the actual amount of cream used for this production. This expression was obtained from a detailed model presented by Corsano et al. [26].

Therefore, the term added to the objective function is:

$$ResC = \sum_{f} (C_{vin}Vres_f + C_{cream}VCres_f)$$
 (71)

where C_{vin} and C_{cream} represent the unit cost for vinasses and centrifuged cream disposals respectively. In this work, these costs are representative values since no appropriate values were found in the literature.

Considering both cost, C_{vin} and C_{cream} , equal to 5 \$/t and the rest of parameters as in case C, the optimal solution is similar to that obtained in case A. Plants f1 and f3 are allocated with the design shown in Fig. 4 and the produced amounts of torula, ethanol and baker's yeast are 18,972 t, 109620 t and 26,790 t respectively for

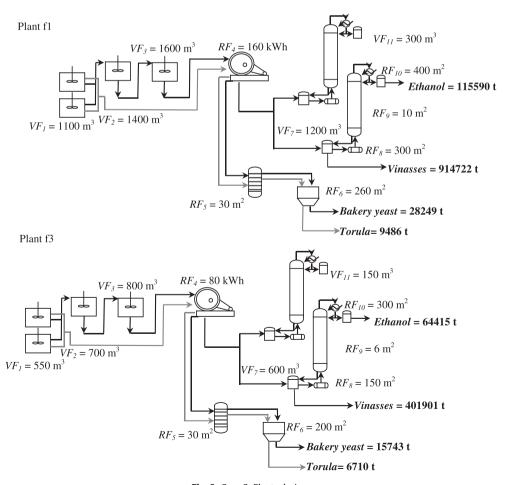


Fig. 6. Case C: Plants design.

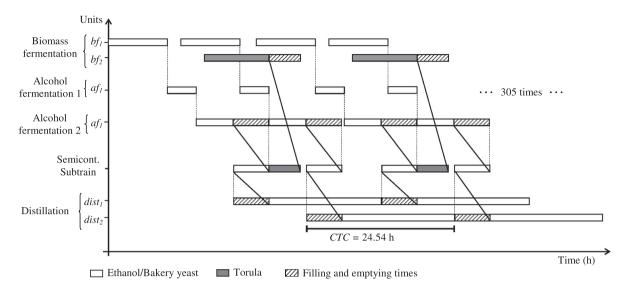


Fig. 7. Case C: Gantt chart for production planning for both plants.

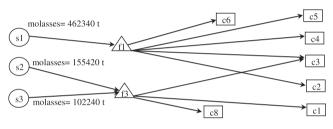


Fig. 8. Case C: SC design.

plant f1, and 13,129 t, 70,380 t and 17,202 t respectively for plant f3. It is worth noting that the produced amount of torula in plant f1 coincides with that in case A. The reason is that the available unit sizes do not allow producing more torula in that plant. In plant f3, the total possible torula is produced according to the unit sizes selected for producing ethanol and baker's yeast, and vinasses are not discarded. The ethanol production is bigger in plant f1 since enough amounts of molasses are available from raw material site s1 (the nearest one). If more ethanol would be produced in plant f3, more molasses would be needed, and therefore the molasses transportation cost would be increased. This means that is more convenient to discard vinasses in plant f1 than process them to produce a larger amount of torula increasing the unit sizes in plant f3 and the transportation costs. Therefore, a clear tradeoff among torula production, unit sizes and transportation cost can be assessed in his case.

The fourth column of Table 8 shows the economical results for this case. It can be observed that the income for sales is greater than in case C since more amount of torula is produced with the aim of decrease the disposal costs.

5. Conclusions

In this article, a MILP formulation for the optimal design of the SC is presented, where not only the allocation of ethanol plants is considered but also detailed formulations for plant design and production planning are included. Previous approaches used to decompose the resolution of these problems in a hierarchical structure. Here a simultaneous formulation is adopted and the different tradeoffs can be assessed. From the planning point of view, several decisions can be chosen, but scheduling with campaigns

was selected taking into account it significantly affects other production issues. Thus, production flows can be determined and, therefore, different operational aspects can be evaluated: transport policy, inventory levels, etc.

The production of yeasts for cattle feeding was incorporated to the model in order to evaluate the benefits of these productions using ethanol residues. Environmental concerns were only considered insofar as they affected the economics of the SC.

The capabilities of the proposed approach were illustrated through several studied cases where different scenarios were analyzed. The presented modeling framework represents a useful tool for decision making and provides valuable insight into the location, design and production planning problem for ethanol and derivative productions and the relationships among these decisions.

Ethanol production is always profitable according to the studied cases, as well as baker's yeast since the unit sizes required to evaporate and dry the fermented broth are not so bigger. However, for torula production, fermentors must to be added and bigger sizes for semicontinuous subtrain are needed. Therefore, if torula selling price is not attractive, its production is not convenient. The plant locations depend on the transportation costs but network flows depend on plant design and production planning, since the amount of each produced product is unknown a priori and they vary according to the proposed scenario. Among the studied cases, the impact of decisions about the impact causes by residue disposal was also considered. Nevertheless, different scenarios can be also studied and new conclusions can be attained. Precisely, the great advantage of the proposed approach is the ability to assess different alternatives.

Numerical results show the importance of simultaneous optimization in this type of problem where several decisions are jointly taken into account and many tradeoffs are together evaluated. As can be observed through the different solved instances, there are effective tradeoffs among the different decisions, and their simultaneous consideration provides a valuable knowledge about the global SC behavior.

This work must be considered from a management perspective, where an appropriate decision making is required. The suitable and simultaneous assessment of the different involved elements must be contemplated. Although a simplified problem description has been presented, the capabilities of the proposed approach can be effectively evaluated. The formulation could be additionally improved from different perspectives to achieve a more realistic problem description. From the SC perspective, new echelons can

be added, including, for example, product warehouses. Process description should consider a more detailed structure. From the operational point of view, logistics could be improved and inventory administration should be incorporated. In this way, the proposed model could be significantly enhanced. From the computational performance standpoint, the problem size and the several evaluations that are simultaneously assessed leads to higher computational burden. Future works will address these limitations and performs new improvements. However, the proposed formulation allows assessing, from a management perspective, the contribution of this kind of mathematical representation that simultaneously evaluate different perspectives usually considered as separated decisions.

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