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Optimal design for sustainable bioethanol supply chain considering detailed plant performance model

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ABSTRACT

The always increasing energy demand combined with the declining availability of fossil fuels is driving forces for the investigation of renewable energy sources. In this context, bioethanol is considered as one of the most appropriate solutions for short term gasoline substitution. Then, the motivation of this work is to propose a MINLP optimization model for a sustainable design and behavior analysis of sugar/ethanol supply chain (SC). A detailed model for ethanol plant design is embedded in the SC model, and therefore plant and SC designs are simultaneously obtained. Yeast production and residue recycles are taken into account in order to assess the environmental impact. The inclusion of sustainability issues in the model produces both economic and operative changes in SC and plant designs. The simultaneous optimization of these elements allows the evaluation of several compromises among design and process variables. These issues are highlighted throughout the evaluated studied cases.

1. Introduction

The world population growth and the higher standards of living are responsible for an always increasing demand of energy. Countries such as China and India with an impressive economy growth have a considerable demand of fossil fuels diminishing its availability. It is expected that the world demand for energy will rise during the next 25 years about sixty percent (Brijder et al., 2005). Against this prospect, biofuels production arises as a good solution to many current economic-environmental problems. Particularly, bioethanol from sugar cane is efficiently produced all over the world and this production does not affect the production of sugar for human consumption, unlike some other raw materials like corn or another biofuel like biodiesel from soybean. Bioethanol is considered as one of the most appropriate solutions for short term gasoline substitution. The most cost-effective scenario, requiring no new technology, is to produce bioethanol from sugar cane at existing facilities extended with a distillery. In order to generate a sustainable and economic production of sugar and bioethanol at the same time, it becomes clear that all related activities such as harvesting, processing and transportation must be organized in a logic and cost effective supply chain optimization model.

Most supply chain (SC) design models have focused on the integration problem, where links among nodes must be settled in order to allow an efficient operation of the whole system in terms of some predefined criteria. Traditionally, the economic benefit has been the most pursued objective in this kind of approaches (Reklaitis & McDonald, 2004; You & Grossmann, 2007). However, in the last five years, there has been a growing interest in incorporating environmental concerns along the traditional economic criteria in the optimization of chemical processes. Hugo and Pistikopoulos (2005) presented a multi-objective optimization problem for the long-range planning and design of SC networks. They incorporated life cycle assessment (LCA) criteria as part of the strategic investment decisions. Guillén and Grossmann (2009) formulated a bi-criterion stochastic mixed-integer nonlinear program (MINLP) for the simultaneous consideration of net present value maximization and environmental impact minimization for chemical SCs in presence of uncertainty. A decomposition approach based on parametric programming is presented for solving the proposed model. Later, they extended this work incorporating another source of uncertainty and developing a modelling framework and solution strategy for the strategic SC management (SCM) problem (Guillén & Grossmann, 2010). Zamboni, Shah, and Bezzo (2009) developed a SC optimization model for bioethanol focused in factories located in the north of Italy. They developed a multi-echelon mixed integer linear program (MILP) model including environmental issues along with the economic ones. Mele, Guillén-Gosálbez, and Jiménez (2009) addressed the SC design for producing sugar and ethanol considering both economical and environmental concerns. They proposed a bi-criterion MILP model that simultaneously minimizes the total network cost and the environmental impact according to the LCA principles. They provided a set of Pareto optimal alternatives for producing sugar and ethanol in the NW region of Argentina.

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Nomenclature

Indices

cen	centrifuge
DFV	distiller feed vessel
dist	distillation
dry	drying
DT	distillate tank
evap	evaporator
ep	ethanol plants
ew	ethanol warehouses
fer	fermentation
fin	final
i	products of sugar plants, *i* = molasses, sugar, electricity
ini	initial
k	customer zones
LO	lower bound
p	final products, *p* = sugar, ethanol, yeast
sp	sugar plants
sw	sugar warehouses
UP	upper bound

Parameters

C_{cen}	centrifuge coefficient
CTr	transportation cost ($ kg^{-1}, $ ton^{-1})
CM_{sp}^{UP}	maximum milled sugar cane for sugar plant *sp* (ton h^{-1})
Dem_{pk}^{LO}	minimum product demand (ton h^{-1}, kg h^{-1})
Dem_{pk}^{UP}	maximum product demand (ton h^{-1}, kg h^{-1})
HT	time horizon (h)
IA_i	conversion factor for product *i* at sugar plant
IC	installation cost ($)
IF	conversion factor for filter juices
IFJ_i	influence factor over product *i* when filter juices are extracted
ks	substrate saturation constant (kg m^{-3})
Os	settled sewage concentration (kg m^{-3})
Q_{ew}^{UP}	maximum ethanol warehouse capacity (kg h^{-1})
Q_{sw}^{UP}	maximum sugar warehouse capacity (ton h^{-1})
SP	selling price ($ kg^{-1}, $ ton^{-1})
U	global transference coefficient (kcal^{-1} m^{-2} $°C^{-1}$)
X^{inoc}	inoculum biomass concentration (kg m^{-3})
Yp	conversion factor biomass-ethanol
Ys	conversion factor biomass-substrate
Z_{BO}	biological oxidation cost ($ m^{-3})
Z_{cream}	centrifuge disposal cost ($ m^{-3})
Z_e	reception and conveyance cost ($ m^{-3})
Z_T	volumetric and primary treatment cost ($ m^{-3})
η	biomass death rate (h^{-1})
μ_{max}	maximum specific growth rate of biomass (h^{-1})
ρ	density (kg m^{-3})
σ_{cen}	centrifuge yield
ΔH	vaporization heat (kcal kg^{-1})
ΔT	difference in temperature (°C)

Variables

A	semicontinuous unit size (m^2)
$Av_{sp,i}$	amount of product *i* produced at sugar plant *sp* (ton h^{-1})
B	ethanol batch size (kg)
CM_{sp}	processed sugar cane at sugar plant *sp* (ton h^{-1})
CT	cycle time (h)
D	duty factor for semicontinuous units
$DispC$	disposal cost ($ h^{-1})
DV	distillery vinasses in inoculation tank (m^3)
DVR	discarded vinasses (m^3)
DVT	total produced vinasses (m^3)
E	ethanol concentration (kg m^{-3})
EFJ_{sp}	percentage of produced filter juices extracted for fermentations (ton h^{-1})
ex_{ep}	binary variable for allocating ethanol plants
FJ_{sp}	produced filter juices at sugar plant *sp* (ton h^{-1})
FJF_{ep}	filter juices consumed at plant *ep* (m^3)
$InsC$	installation cost ($ h^{-1})
$InvC$	investment cost ($ h^{-1})
IS	sale income ($ h^{-1})
M_{ep}	molasses consumed at plant *ep* (m^3)
ND	number of out of phase distillation units
NF	number of out of phase fermentors
NP	net profit ($ h^{-1})
OC	operating cost ($ h^{-1})
Q	flow rate (kg h^{-1})
Rc	centrifuge power (kWh)
S	substrate concentration (kg m^{-3})
t	processing time (h)
TrC	transportation cost ($ h^{-1})
V	volume (m^3)
VL	evaporator inlet volume (m^3)
VR	centrifuge residue volume (m^3)
VT	inoculation tank size (m^3)
VF	fermentor size (m^3)
Wat_{ep}	fresh water consumed at plant *ep* (m^3)
we	binary variable for allocating ethanol warehouses
ws	binary variable for allocating sugar warehouses
X	biomass concentration (kg m^{-3})
$x_{d,ep}$	binary variable for selecting number of parallel units at distillation stage
$x_{m,ep}$	binary variable for selecting number of parallel units at fermentation stage
Xd	non-active biomass concentration (kg m^{-3})
μ_{ep}	specific growth rate of biomass (h^{-1})

It is worth mentioning that in all previous cited works, facility performance models was not taken into account, and the plants involved in the SC were simplified models. Generally, decision making about plant structures is delayed until SC is configured. Shah (2005) points out that both the network and the individual units conforming the SC must be designed appropriately. He also emphasizes that there are potential tradeoffs to be exploited. Despite the extensive background about SC optimization (Goetschalckx, Vidal, & Dogan, 2002; Shah, 2005; Shapiro, 2004; Varma, Reklaitis, Blau, & Penky, 2007), there are few published works about the integration of different SC decision levels. Naraharisetti, Karimi, and Srinivasan (2008) considered a multi-echelon supply chain network of a multi-national corporation and presented a deterministic asset management model. They also combined both the strategic (facility planning) and tactical asset management (production–allocation–distribution) problems into an integrated asset management, capital budgeting, and supply chain redesign model. Amaro and Barbosa-Póvoa (2008) presented a MILP model for the detailed optimal scheduling of SC where operational decisions are explicitly integrated. Puigjaner, Laínez, and Álvarez (2009) presented a SC design-planning model coupling with a scheduling formulation, so that decision levels integration is achieved. This approach allows assessing the impact of considering scheduling aspects of process operations in the design of a supply chain network. In a recent work, Corsano and Montagna (2011) presented a model for the simultaneous optimization of SC and plant designs. They showed that the incorporation of plant design into the SC design model obtained better solutions which differ notably from the sequential or hierarchical approaches, both in economic values and SC structure. However, they considered a very simple model, with fixed processing times and fixed size factors for processing units.

Ethanol production has become one of the most important alternatives for the production of renewable biofuel owing to its compatibility with the supply chain of gasoline and its capability of being readily used in the current design of automobiles (Cole, 2007). In last years, several authors have addressed the production of ethanol from different raw materials. Karuppiah et al. (2008) addressed the design and energy optimization for corn-based ethanol plants. They proposed superstructure optimization approach where the optimal plant design is obtained decoupling a MINLP model into two non-linear programming (NLP) subproblems. Then, they perform the heat integration analysis for the resulting process. The authors showed that it is possible to reduce the current steam consumption by more than 40% compared to initial basic design. Martín and Grossmann (2010) presented the superstructure optimization for bioethanol production via gasification of lignocellulosic material like switchgrass. They modeled the process as an MINLP using short-cut methods for each unit operation. The superstructure is optimized for minimum required energy and then, economic evaluation of the options is used to select the most profitable process. Other authors (Hosseini and Shah, 2009; Corsano, Iribarren, Montagna, Aguirre, & González Suárez, 2006) have also addressed the problem of ethanol production through mathematical programming formulations.

For a sustainable integration of the bioethanol supply chain the attention must be focused on by-products of sugar and ethanol factories. In this sense, sugar production generates molasses and filter juices which both serve as sugaring substrate for ethanol. Another important sugar secondary product is electricity that can be supplied to power networks or to ethanol plants. On the other hand, bioethanol process generates a non-distilled remainder called vinasses. Because of pollution problems, the treatment of vinasses is one of the most significant and challenging issues in the industrial production of ethanol. Usually, vinasses are discarded causing a considerable environmental impact. Another vinasses characteristic is its fast degradation and, thus, its storage is not recommended. A sustainable alternative for ethanol production is the recycling of vinasses to fermentation stage of the same ethanol plant. In this way, vinasses contribute to the sugaring substrate for fermentation. In addition, the centrifuge residue, which is a cream with considerable biomass concentration, is generally discarded, causing direct soil pollution where it is disposed. The treatment of this residue consists of processing it for producing yeast for cattle feeding. In a previous article Corsano et al. (2006), presented a mathematical model for the optimal synthesis, design and operation of an ethanol plant considering the environmental impact caused by the process waste disposals. They analyzed several plant designs and operation scenarios for different disposal policies.

In this work, a MINLP model is proposed for the SC of bioethanol production from sugar cane. The optimization model is composed of several sugar and ethanol plants, ethanol warehouses and customer regions. A detailed formulation for ethanol plants is embedded in the overall SC model to perform the sustainability analysis. Therefore, it is possible to explore the SC design and behavior according to the amount of molasses, filter juices and electricity provided to ethanol production plants which can affect the sugar production. It is also viable to examine the effect of vinasses recirculation from downstream stages in ethanol plants and the production of yeast for cattle feeds. The inclusion of all these details in a high level performance model for the ethanol plants allows the sustainability analysis which cannot be done without its consideration. Some other matters are also posed in this formulation, since the number of ethanol plants and its location is determined by this model, transportation cost between sugar–plants/ethanol–plants/ethanol–warehouses/customer-regions are included on it. As a consequence, several tradeoffs arising with the simultaneous optimization are solved with the proposed approach, which is not frequently found in the literature of this area.

The capability of the presented formulation is highlighted through the solution of different scenarios assessing diverse environmental and economic assumptions. Different disposal costs are proposed in order to explore the SC design and behavior in different examples. The results obtained are shown at the end of this article. The proposed model represents a tool for providing decision-support for different sustainable production–distribution systems of ethanol from sugar cane.

2. Problem definition

In this work a SC involving raw material sites, production plants, warehouses and customer zones is considered. Fig. 1 shows the proposed SC echelons and possible links.

The raw material sites consist of a set of N_{SP} existing sugar plants, each one with capacity for processing at most CM_{sp}^{UP} tons per hour of sugar cane. The amount of processed sugar cane is an optimization variable and it is assumed that this raw material is available near to the sugar plant and no cane transportation cost is considered in the model. The sugar plants produce sugar for sale, and molasses, filter juices, and electricity are available for ethanol production. Molasses are a by-product of the sugar process and its production does not affect the amount of produced sugar. Filter juices are an intermediate flow of the sugar process and it can be extracted to be used for ethanol production or can be recycled to the sugar process. If filter juices are extracted the amounts of produced sugar and molasses are decreased while the amount of electricity available is increased. When filter juices are recycled to sugar process bigger amount of sugar and molasses are produced, but more electricity is consumed in the process decreasing the extra-factory electricity availability. In this way, the amounts of produced sugar, molasses and electricity are optimization variables depending on amount of processed sugar cane and extracted filter juices. Therefore, there is a compromise between the produced sugar, molasses, and electricity against filter juice extraction.

Molasses and filter juices are transported from sugar to ethanol plants. They are used as sugaring substrate for fermentation process. Electricity is used by the centrifuges of ethanol process and the amount not consumed is sold to the electricity network. If the available electricity is not enough for ethanol plant demands, it is bought from the network and its cost is imputed in the model.

The produced sugar is delivered to sugar warehouses. Each sugar warehouse sw ($sw = 1, \ldots, N_{SW}$) has limited capacity, Q_{sw}^{UP}. If produced sugar is bigger than its demands, the excess can be exported to other customer zones with lower prices.

There are up to N_{EP} ethanol plants that can produce ethanol and yeast for cattle feeding. The design of ethanol plants is simultaneously decided with SC design. Fig. 2 shows a flowsheet for an ethanol plant. The plant stages are inoculum preparation, where the inoculum is mixed with the molasses, filter juice, vinasses and fresh water, fermentation, centrifugation, and distillation for producing ethanol. For producing yeast from the centrifugation residue, a semicontinuous evaporator and a dryer are used. Yeast

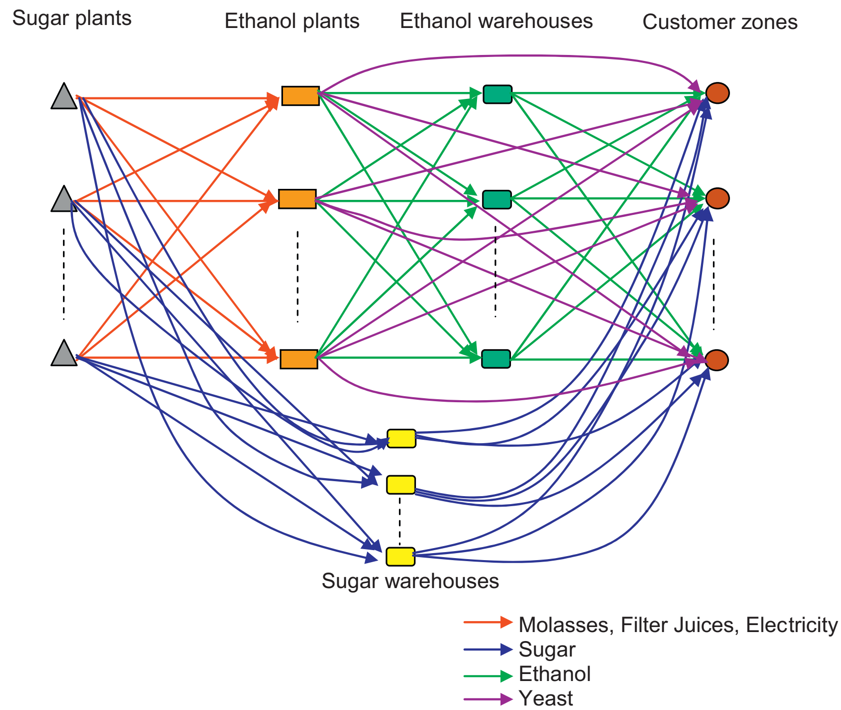

Fig. 1. SC design.

production is optional and the residual broth of the centrifuge can be partially or totally discarded. If centrifuge cream residue is discarded, a disposal cost is imputed according to the discarded volume. For fermentation and distillation stages, the number of out of phase parallel units used in each ethanol plant is an optimization decision. Each ethanol plant generates a non-distilled remainder called vinasses or distillery broth that can represent another substrate contribution for fermentations. Due to vinasses degradation, they cannot be transported and therefore, they are recycled to the same plant. The vinasses recycle and its substrate concentration is a model decision and if they are discarded, a penalty is added in the objective function according to the disposal volume and concentration. But if vinasses are used in fermentation, the volume of inoculation tank is increased and the blend is more diluted since the vinasses substrate concentration is upper bounded by $10\,g\,l^{-1}$. Therefore, there is a tradeoff between vinasses recycle and unit sizes, or in other words, between disposal cost and investment cost. The ethanol plant design, embedded in the overall SC design formu-

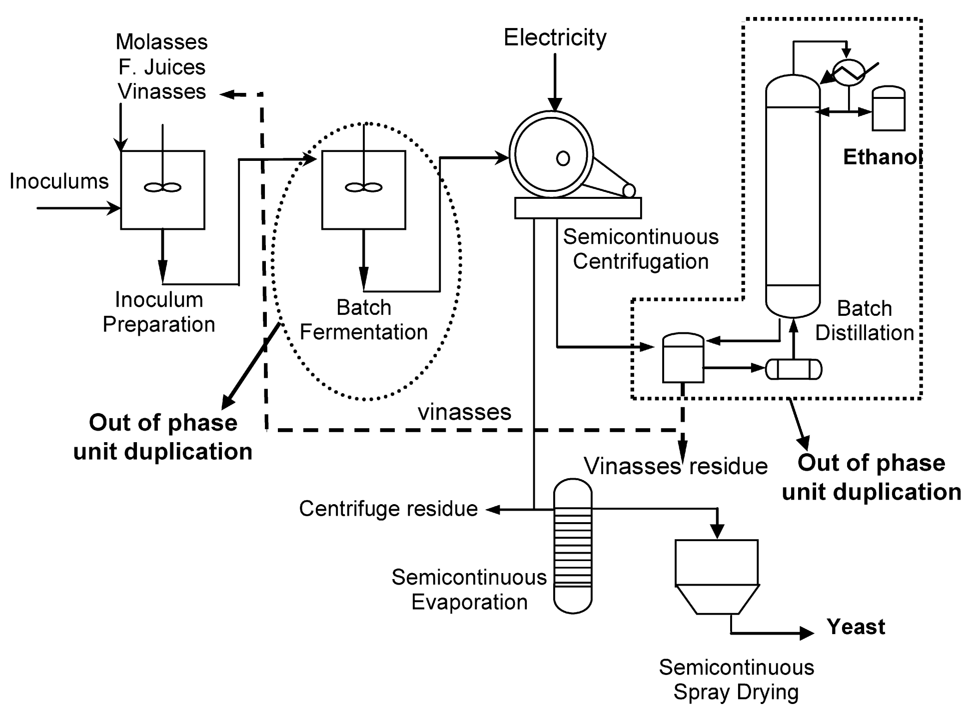

Fig. 2. Ethanol plant flowsheet.

lation, is a detailed model including design and operating variables like inoculums, processing times, material concentrations, etc.

The produced yeast is directly transferred to the customers because its degradation is fast (72 h approximately), while the ethanol is delivered to ethanol warehouses. There are up to N_{EW} ethanol warehouses to be allocated, each one with limited capacity given by Q_{ew}^{UP} for $ew = 1, \ldots, N_{EW}$.

At each customer zone k ($k = 1, \ldots, N_K$), there are minimum (Dem_{pk}^{LO}) and maximum (Dem_{pk}^{UP}) demands of final products p that must be fulfilled (p = sugar, ethanol, yeast).

In short, the SC and plant design problem consists in determining simultaneously:

- The amount of processed milled cane (CM_{sp}), such that $CM_{sp} \leq CM_{sp}^{UP}$
- The produced amounts in each sugar plant: sugar, molasses, filter juices, and electricity.
- The ethanol plants to be allocated.
- The amounts of produced ethanol and yeast.
- The configuration of ethanol plants and the unit sizes.
- The vinasses recycle and yeast production in order to reduce the environmental impact caused by their disposals.
- The sugar and ethanol warehouses to be allocated.
- The material flows among SC nodes.

The objective is to maximize the total benefits given by product sales minus installation, investment, logistic and disposal costs.

3. Model formulation

The problem involves optimizing the SC design simultaneously with the ethanol plant designs in order to obtain a profitable and sustainable process and network integration. With the simultaneous optimization, all the tradeoffs between plants and supply chain decisions can be considered and assessed. Following, the basic constraints are posed and the definition of variables and parameters are presented in Nomenclature.

3.1. Sugar cane plant constraints

The amount of sugar cane processed at plant sp is bounded by

$$CM_{sp} \leq CM_{sp}^{UP} \quad sp = 1, \ldots, N_{SP} \tag{1}$$

The sugar cane plants can produce sugar, molasses, and electricity according to the processed sugar cane and the amount of extracted filter juices. The filter juices are produced in the sugar plant and they can be extracted for fermentation process of ethanol plants or can be recycled to the sugar process. The total amount of produced filter juices, FJ_{sp}, is given by

$$FJ_{sp} = CM_{sp} IF \quad sp = 1, \ldots, N_{SP} \tag{2}$$

where IF is a conversion factor equal to 0.1152.

The filter juices can be partially or totally recycled to sugar process, and the amount of sugar, molasses and electricity produced in each sugar plant ($Av_{sp,i}$) depends on the percentage of produced filter juices extracted for fermentation processes, EFJ_{sp} ($0 \leq EFJ_{sp} \leq 1$). The tons per hour of product i (i = sugar, mol, elect) produced in each sugar plant sp are

$$Av_{sp,i} = CM_{sp} IA_i - FJ_{sp} EFJ_{sp} IFJ_i \quad sp = 1, \ldots, N_{sp},$$
$$i = \text{sugar, mol, elect} \tag{3}$$

where IA_i is the conversion factor for the production of product i in the sugar plant and IFJ_i the coefficient that indicates how the extraction of filter juices affects to the production of product i. In this way, if filter juices are totally recycled to sugar process, then EFJ_{sp} is equal to zero and the produced sugar, molasses and electricity depend on the processed milled cane. The values for IA_i and IFJ_i are shown in Table 1. The coefficient IFJ_i for electricity is negative since the available electricity is increased when filter juices are extracted (Eq. (3)). These parameters values, as well as IF factor, were obtained from experimental industrial data and assessed with values found in the literature (Mele et al., 2009). It is worth mentioning that these parameters can vary according to different technologies utilized in the sugar cane production processes, as was presented by Kostin, Guillén-Gosálbez, Mele, Bagajewicz, and Jiménez (2010).

Table 1
Conversion factors and filter juices influence coefficients.

	Sugar	Molasses	Electricity
IA_i	0.115	0.04	0.985
IFJ_i	0.085	0.02	−20.0

3.2. Ethanol plants constraints

There are up to N_{EP} ethanol plants to be allocated in the SC. The stages of the ethanol plants are showed in Fig. 2. Following, mass balances between stages and design equations for each unit are posed

3.2.1. Inoculation preparation

The inoculum is blended with molasses and filter juices provided by the sugar cane plants, fresh water, and vinasses from the same ethanol plant. The amount of inoculum is a process variable with biomass concentration equal to 40 g l^{-1}. The mass balances for this stage are:

$$VT_{ep} = V_{ep}^{inoc} + M_{ep} + FJF_{ep} + DV_{ep} + Wat_{ep} \quad \text{for} \quad ep = 1, \ldots, N_{EP} \tag{4}$$

where V_{ep}^{inoc}, M_{ep}, FJF_{ep}, DV_{ep}, Wat_{ep} represent the volume of inoculum, molasses, filter juices, distillery vinasses and fresh water respectively, that are blended in plant ep. VT_{ep} is the inoculum tank size.

3.2.2. Fermentation

The fermentation stage is modeled according to the formulation presented in Corsano, Aguirre, Iribarren, and Montagna (2004) which considers the following differential equations using Monod's kinetics model:

$$\frac{dX_{ep}}{dt_{fer,ep}} = (\mu_{ep} - \eta) X_{ep} \quad ep = 1, \ldots, N_{EP} \tag{5}$$

$$\frac{dS_{ep}}{dt_{fer,ep}} = -\frac{\mu_{ep}}{Ys} X_{ep} \quad ep = 1, \ldots, N_{EP} \tag{6}$$

$$\frac{dE_{ep}}{dt_{fer,ep}} = \frac{\mu_{ep}}{Yp} X_{ep} \quad ep = 1, \ldots, N_{EP} \tag{7}$$

$$\frac{dXd_{ep}}{dt_{fer,ep}} = \eta X_{ep} \quad ep = 1, \ldots, N_{EP} \tag{8}$$

with

$$\mu_{ep} = \frac{\mu_{\max}}{ks + S_{ep}} S_{ep} \quad ep = 1, \ldots, N_{EP} \tag{9}$$

X, S, E, and Xd are the biomass, substrate, ethanol, and non-active biomass concentration respectively. $t_{fer,ep}$ is the processing time for fermentation stage of plant ep, and η is biomass death rate. The yield coefficient, Ys, which is an efficiency measure for a particular conversion, in this case the substrate-biomass conversion, is taken equal to 0.124 while the substrate-ethanol yield coefficient

Yp is considered as 0.23. ks is substrate saturation constant equal to 20 kg m^{-3} and $\mu_{\max}$ is maximum specific growth rate of biomass equal to 0.1 h^{-1}. The model parameters were experimentally found and reported by De la Cruz Soriano et al. (2003) and they depend on the carbohydrate source.

The differential equations are discretized and embedded into the model as algebraic equations (Corsano et al., 2004).

The mass balances between inoculum tank and fermentor for each component are

Biomass:

$$X^{inoc}V^{inoc}_{ep} = X^{ini}_{ep}VF_{ep} \quad ep = 1,\ldots,N_{EP} \tag{10}$$

where X^{inoc} is the inoculum biomass concentration equal to 40 g l^{-1}.

Substrate:

$$S_M M_{ep} + S_{FJ}FJ_{ep} + S_{DV,ep}DV_{ep} = S^{ini}_{ep}VF_{ep} \quad ep = 1,\ldots,N_{EP} \tag{11}$$

It is worth mentioning that vinasses substrate concentration, $S_{DV,ep}$, is a process variable, while S_M and S_{FJ} are model parameters equal to 779.6 g l^{-1} and 100 g l^{-1} respectively. Therefore, there is a tradeoff between vinasses substrate concentration and fermentation processing time, since long fermentation implies lower substrate concentration. A detailed analysis about this issue was presented by Corsano et al. (2006).

Volume:

$$VT_{ep} = VF_{ep} \quad ep = 1,\ldots,N_{EP} \tag{12}$$

From the discretization of Eqs. (5)–(9), the initial ($X^{ini}_{ep}, S^{ini}_{ep}, E^{ini}_{ep}, Xd^{ini}_{ep}$) and final ($X^{fin}_{ep}, S^{fin}_{ep}, E^{fin}_{ep}, Xd^{fin}_{ep}$) concentrations of each component and the processing time for fermentation stage $t_{fer,ep}$ are obtained. Then, the following specification constraints are stated:

$$S^{ini}_{ep} = S^{UP}_{ep}ex_{ep} \quad ep = 1,\ldots,N_{EP} \tag{13}$$

$$X^{fin}_{ep} \geq X^{LO}_{ep}ex_{ep} \quad ep = 1,\ldots,N_{EP} \tag{14}$$

$$E^{fin}_{ep} \geq E^{LO}_{ep}ex_{ep} \quad ep = 1,\ldots,N_{EP} \tag{15}$$

$$E^{ini}_{ep} = 0 \quad ep = 1,\ldots,N_{EP} \tag{16}$$

$$VT_{ep} \leq VT^{UP}_{ep}ex_{ep} \quad ep = 1,\ldots,N_{EP} \tag{17}$$

$$V^{inoc}_{ep} \leq \tfrac{3}{4}VT^{UP}_{ep}ex_{ep} \quad ep = 1,\ldots,N_{EP} \tag{18}$$

where $ex_{ep} = \begin{cases} 1 & \text{if ethanol plant } ep \text{ is allocated} \\ 0 & \text{otherwise} \end{cases}$

The superscripts LO and UP represent lower and upper bounds parameters. In this way, the above constraints state bounds or conditions for product components if the plant is allocated or force them to be zero otherwise. Eq. (13) imposes the initial substrate concentration equal to the maximum substrate concentration since the substrate is consumed in this stage. Eqs. (14) and (15) require biomass and ethanol concentrations bigger than the minimum allowed value. Eq. (16) forces to be zero the initial ethanol concentration since inoculum does not contain ethanol. Eqs. (17) and (18) limit the inoculation tank size and the utilized inoculum.

3.2.3. Centrifugation

The biomass separation, previous to the distillation, is performed in a semicontinuous disks stack centrifuge. The design equation for this semicontinuous unit is:

$$Rc_{ep} = Dc_{ep}\frac{VF_{ep}}{t_{cen,ep}} \quad ep = 1,\ldots,N_{EP} \tag{19}$$

where Rc_{ep}, Dc_{ep}, $t_{cen,ep}$ are the centrifuge size in power units, the centrifuge duty factor, and the processing time respectively. The duty factor is estimated by:

$$Dc_{ep} = \frac{K_C}{\sigma_{cen}} \quad ep = 1,\ldots,N_{EP} \quad \text{where} \quad K_C = \frac{K}{\nu_g} = 0.5\,\text{kW m}^{-3}\,\text{h} \tag{20}$$

σ_{cen} is the centrifuge yield measured as the ratio of biomass separated to total biomass present in the feed equal to 0.85, K is a constant that depends on the centrifuge type and ν_g is the terminal settling velocity of the particles in a gravitational field. K_C was calculated from data reported by Petrides, Sapidou, and Calandranis (1995) for *Escherichia coli*, accounting for the relative size between yeast and *E. coli*.

The volume entering into the centrifuge is equal to the fermentation volume VF_{ep}, and the volume that exits from the centrifuge to distillation stage is VC_{ep}. The centrifuge residual is a cream that can be partially or totally processed for producing yeast. The volume used for producing yeast is VL_{ep} while the disposal volume is VR_{ep}. Therefore, taking into account that C_{cen} is the centrifuge concentration factor, the volume balances between fermentation and centrifugation stages are:

$$VC_{ep} = (1 - C_{cen})VF_{ep} \quad ep = 1,\ldots,N_{EP} \tag{21}$$

$$VL_{ep} + VR_{ep} = C_{cen}VF_{ep} \quad ep = 1,\ldots,N_{EP} \tag{22}$$

The discarded volume (VR_{ep}) is penalized in the objective function. A sustainable solution is to produce yeast for cattle feeding with centrifuge residual. If the disposal cost is high, the volume processed for producing yeast is increased and therefore, the size for the down stream units (evaporator and dryer) is also increased. Therefore, there is a tradeoff between disposal cost and investment costs of evaporation and drying stages.

Finally, at this stage the metabolite and substrate concentrations do not change, but the biomass balances between centrifugation and fermentation stages are:

$$X^{cen}_{ep}(VL_{ep} + VR_{ep}) = \sigma_{cen}(X^{fin}_{ep} + Xd^{fin}_{ep})VF_{ep} \quad ep = 1,\ldots,N_{EP} \tag{23}$$

3.2.4. Evaporation

For producing yeast, the centrifuge residue, or part of it, is evaporated and then dried. If no yeast is produced, then the total centrifuge residue is discarded and evaporator and dryer are not installed.

If yeast is produced, the evaporator inlet flow is equal to VL_{ep}, while the biomass concentration is equal to X^{cen}_{ep}, then the biomass balance in evaporation stage is:

$$VL_{ep}X^{cen}_{ep} = V^{evap}_{ep}X^{evap}_{ep} \quad ep = 1,\ldots,N_{EP} \tag{24}$$

The evaporator is a semicontinuous item and its design is given through its area:

$$A^{evap}_{ep} = \frac{D^{evap}_{ep}W^{evap}_{ep}}{t_{evap,ep}} \quad ep = 1,\ldots,N_{EP} \tag{25}$$

with D^{evap}_{ep} the given duty factor calculated by

$$D^{evap}_{ep} = \frac{\Delta H}{U_{evap}\Delta T} \quad ep = 1,\ldots,N_{EP} \tag{26}$$

The design parameters $\Delta H = 540$ kcal kg^{-1}, $U_{evap} =$ 675 kcal (h m^2 °C)$^{-1}$, and $\Delta T = 70$ °C, are the standard heat of vaporization, the heat transfer coefficient, and the temperature difference respectively (Douglas, 1988). W^{evap}_{ep} represents the kilograms of evaporated water in this stage which is estimated as $100(V^{evap,in}_{ep} - V^{evap}_{ep})$, and $t_{evap,ep}$ is the evaporation processing time.

3.2.5. Drying

The evaporated cream is then dried for obtaining yeast with a specified biomass concentration X_{ep}^{dry} of 1004.6 kg m^{-3} (8% moisture).

The mass balances for this stage is:

$$V_{ep}^{evap}X_{ep}^{evap} = V_{ep}^{dry}X_{ep}^{dry} \quad ep = 1, \ldots, N_{EP} \tag{27}$$

The unit size is calculated through its area:

$$A_{ep}^{dry} = \frac{D_{ep}^{dry}W_{ep}^{dry}}{t_{dry,ep}} \quad ep = 1, \ldots, N_{EP} \tag{28}$$

where D_{ep}^{dry} is the dryer duty factor calculated by means of Eq. (29), W_{ep}^{dry} represents the kilograms of dried water in this stage which is estimated as $100(V_{ep}^{evap} - V_{ep}^{dry})$ and $t_{dry,ep}$ is the processing time for the drying.

$$D_{ep}^{dry} = \frac{\Delta H}{U_{dry}\Delta T} \quad ep = 1, \ldots, N_{EP} \tag{29}$$

The design parameters ΔH and ΔT are the same adopted for evaporation stage while U_{dry} is equal to 35 kcal (h m^2 °C)$^{-1}$.

The yeast is obtained in this stage and the production equation is given by

$$Q_{ep}^{yeast} = \frac{X_{ep}^{dry}V_{ep}^{dry}}{CT_{ep}} \quad ep = 1, \ldots, N_{EP} \tag{30}$$

where Q_{ep}^{yeast} represents the kilograms per hour of yeast produced at plant *ep*. CT_{ep} is the plant cycle time and will be defined in the scheduling constraints section.

3.2.6. Distillation

The analytical process performance model presented by Zamar, Salomone, and Iribarren (1998) and adapted for ethanol production by Corsano et al. (2006) for batch distillation was adopted, where the size of distillation items depends on the value of two process optimization variables: the internal reflux ratio and the number of separation stages. The detailed formulation is not presented in this paper because of space reasons. As it is shown in Fig. 2, the batch distiller is a combination of two batch items: the distiller feed vessel and the distillate tank, and three semicontinuous items: the evaporator, the condenser and the column itself.

The ethanol production is obtained from the distillate tank and is equal to

$$Q_{ep}^{eth} = \frac{B_{ep}}{CT_{ep}} \quad ep = 1, \ldots, N_{EP} \tag{31}$$

where B_{ep} is the ethanol batch size. On the other hand, the produced vinasses are obtained from the distiller feed vessel and they can be recycled to the inoculation tank or can be discarded. The residual vinasses, DVR_{ep}, are calculated as

$$DVR_{ep} = DVT_{ep} - DV_{ep} \quad ep = 1, \ldots, N_{EP} \tag{32}$$

where DVT_{ep} are the total produced vinasses and DV_{ep} are the vinasses recycled to the inoculation tank.

The vinasses substrate concentration is a process variable and it depends on the fermentation processing time, since the substrate is consumed in that stage. Therefore, for longer processing time, lower vinasses substrate concentration is reached. The vinasses substrate concentration is upper bounded by 10 g l^{-1}. The vinasses disposal is penalized in the objective function. On the other hand, if vinasses are recycled to the inoculation tank, its unit size is increased and the inoculum is diluted because vinasses substrate concentration is lower than molasses and filter juice substrate concentration. Therefore, there are several compromises between recycle and disposal decisions.

3.2.7. Timing constraints

Due to the model characteristics and the biomass degradation in the fermentation stage, the most appropriate transfer policy is zero wait (ZW), where the batch processed in a unit is immediately transferred to the following one.

It must be noted that in this model stage processing times are optimization variables and they are obtained from detailed submodels, some of them written as differential equations and included in the overall model. Therefore, the simultaneous optimization allows the evaluation of several tradeoffs including timing variables.

When a batch unit is located between semicontinuous units, the time that the batch unit will be occupied considers the material loading time from the previous semicontinuous unit and unloading time for the next semicontinuous unit.

In this approach, unit duplication is considered for batch stages (fermentation and distillation). Let NF_{ep} and ND_{ep} be the number of out of phase units for fermentation and distillation stages for each ethanol plant *ep*, NF_{ep}^{UP} and ND_{ep}^{UP} represents the maximum number of allowable parallel units for fermentation and distillation stages respectively, and $x_{m,ep}$ and $x_{d,ep}$ the binary variables defined by

$$x_{m,ep} = \begin{cases} 1 & \text{if fermentation stage has } m \text{ unit out of phase} \\ 0 & \text{otherwise} \end{cases} \tag{33}$$

$$x_{d,ep} = \begin{cases} 1 & \text{if distillation stage has } d \text{ unit out of phase} \\ 0 & \text{otherwise} \end{cases} \tag{34}$$

Then,

$$NF_{ep} = \sum_{m=1}^{NF_{ep}^{UP}} m x_{m,ep} \quad ep = 1, \ldots, N_{EP} \tag{35}$$

$$ND_{ep} = \sum_{d=1}^{ND_{ep}^{UP}} d\, x_{d,ep} \quad ep = 1, \ldots, N_{EP} \tag{36}$$

$$\sum_{m=1}^{NF_{ep}^{UP}} x_{m,ep} = ex_{ep} \quad ep = 1, \ldots, N_{EP} \tag{37}$$

$$\sum_{d=1}^{ND_{ep}^{UP}} x_{d,ep} = ex_{ep} \quad ep = 1, \ldots, N_{EP} \tag{38}$$

In this way, the fermentation cycle time is calculated through the expression:

$$CT_{fer,ep} = \frac{t_{fer,ep} + t_{cen,ep}}{NF_{ep}} \quad ep = 1, \ldots, N_{EP} \tag{39}$$

and the distillation cycle time is:

$$CT_{dist,ep} = \frac{t_{dist,ep} + t_{cen,ep}}{ND_{ep}} \quad ep = 1, \ldots, N_{EP} \tag{40}$$

The centrifugation, evaporation and drying stages are semicontinuous. Several consecutive semicontinuous units give rise to a semicontinuous subtrain. In this paper, only perfectly synchronized subtrains are considered, then:

$$t_{cen,ep} = t_{evap,ep} = t_{dry,ep} \quad ep = 1, \ldots, N_{EP} \tag{41}$$

Therefore, the plant cycle time is determined as the maximum stage cycle time of the plant:

$$CT_{ep} = \max\{CT_{fer}, CT_{dist}, t_{cen}\} \quad ep = 1, \ldots, N_{EP} \tag{42}$$

Eq. (42) was reformulated in order to avoid a discontinuous MINLP by substituting "≥" constraints for "max" functions.

3.3. SC design constraints

These constraints are material balances among the different nodes in the SC, and energy balances between sugar plants and ethanol plants.

Following, the constraints between different SC nodes are formulated:

3.3.1. Mass balances between sugar plants and ethanol plants

The connections between sugar and ethanol plants are given by molasses, filter juices and electricity.

Let $Q^{mol}_{sp,ep}$ be the amount per hour of molasses from sugar plant sp to ethanol plant ep. Then the molasses balances are:

$$Av_{sp,mol} \geq \sum_{ep=1}^{N_{EP}} Q^{mol}_{sp,ep} \quad sp = 1, \ldots, N_{SP} \tag{43}$$

$$\sum_{sp=1}^{N_{SP}} Q^{mol}_{sp,ep} = \frac{M_{ep}\rho_{mol}}{CT_{ep}} \quad ep = 1, \ldots, N_{EP} \tag{44}$$

Eq. (43) poses that molasses from each sugar plant must not exceed the produced molasses. ρ_{mol} represents the molasses density and it is used in Eq. (44) because M_{ep} is expressed in volume unit. This equation states that the amount of molasses received from the sugar plants to each ethanol plant is equal to the consumed molasses at fermentation stage of plant ep.

Similar constraints are stated for filter juice balances. Molasses that are not consumed in the ethanol plant can be sold as a nutrient for cattle feeding, but in this approach the surplus of molasses is not considered. As filter juices can be recycled to sugar processes to produce more sugar and molasses, there is not a surplus of filter juice.

The electricity consumed by the ethanol plant corresponds to the power of the centrifuge, Rc_{ep}. If the electricity produced in the sugar plants is not enough to satisfy ethanol plant demands, it is bought from the electricity network. On the other hand, if electricity produced is bigger than the ethanol plant demands, the remainder is sold to the local power network.

The energy balances between sugar plants and ethanol plants are:

$$Av_{sp,elec} - \sum_{ep=1}^{N_{EP}} Q^{elec}_{sp,ep} - Q^{ex\_elec}_{sp} = 0 \quad sp = 1, \ldots, N_{SP} \tag{45}$$

$$\sum_{sp=1}^{N_{SP}} Q^{elec}_{sp,ep} = Rc_{ep} \quad ep = 1, \ldots, N_{EP} \tag{46}$$

$Q^{ex\_elec}_{sp}$ is a non-sign restrictive variable denoting the imported or exported electricity. If it is positive represents the exported electricity and becomes an income in the objective function, otherwise it is bought from the network representing a cost term in the objective function. $Q^{elec}_{sp,ep}$ is the consumed electricity in plant ep and Eq. (46) indicates the balance between sugar and ethanol plant.

3.3.2. Mass balances between sugar plants and sugar warehouses

The produced sugar can be sent to warehouses in order to fulfill the customer zone demands or can be exported with a lower price to other customers. Let $Q^{sugar}_{sp,sw}$ be the sugar produced at sp sugar plant and sent to sw sugar warehouse, and let $Q^{ex\_sugar}_{sp}$ the sugar exported to other markets, then the sugar balance is expressed by Eq. (47).

$$Av_{sp,sugar} = \sum_{sw=1}^{N_{SW}} Q^{sugar}_{sp,sw} + Q^{ex\_sugar}_{sp} \quad sp = 1, \ldots, N_{SP} \tag{47}$$

Each sugar warehouse is limited in capacity, and Q^{UP}_{sw} represents the upper bound for the stored sugar at sw. Then, sugar warehouses capacity is expressed by

$$\sum_{sp=1}^{N_{SP}} Q^{sugar}_{sp,sw} \leq Q^{UP}_{sw} ws_{sw} \quad sw = 1, \ldots, N_{SW} \tag{48}$$

where ws_{sw} is the binary variable equal to 1 if sugar warehouse ws is installed or zero otherwise.

3.3.3. Mass balances between sugar warehouses and customer zones

There are minimum and maximum demands that must be fulfilled:

$$\sum_{sw=1}^{N_{SW}} Q^{sugar}_{sw,k} \geq Dem^{LO}_{sugar,k} \quad k = 1, \ldots, N_K \tag{49}$$

$$\sum_{sw=1}^{N_{SW}} Q^{sugar}_{sw,k} \leq Dem^{UP}_{sugar,k} \quad k = 1, \ldots, N_K \tag{50}$$

There is not stock accumulation at sugar warehouses, therefore all the sugar sent from sugar plants to warehouse sw is then delivered to customer zones.

$$\sum_{sp=1}^{N_{SP}} Q^{sugar}_{sp,sw} = \sum_{k=1}^{N_K} Q^{sugar}_{sw,k} \quad sw = 1, \ldots, N_{SW} \tag{51}$$

3.3.4. Mass balances between ethanol plants and ethanol warehouses

The produced amount of ethanol $Q^{eth}_{ep} = (B_{ep}/CT_{ep})$ at plant ep is transferred to ethanol warehouse ew:

$$Q^{eth}_{ep} = \sum_{ew=1}^{N_{EW}} Q^{eth}_{ep,ew} \quad ep = 1, \ldots, N_{EP} \tag{52}$$

The ethanol warehouses have a limited capacity, therefore defining we_{ew} as the binary variable equal to 1 if ethanol warehouse ew is allocated and zero otherwise:

$$\sum_{ep=1}^{N_{EP}} Q^{eth}_{ep,ew} \leq Q^{UP}_{ew} we_{ew} \quad ew = 1, \ldots, N_{EW} \tag{53}$$

The capacity for each ethanol plant is given by the unit sizes and units duplication. These are problem decisions and it is difficult to determine a priori an upper bound for plant capacity through these variables. But, according to the maximum ethanol demands, a reasonable upper bound for ethanol production in each plant is $Q^{UP}_{ep} = \sum_{k=1}^{N_K} D^{UP}_{eth,k}$. Then, in order to reduce the search space, the following constraint is stated:

$$Q^{eth}_{ep,ew} \leq Q^{UP}_{ep} ex_{ep} \quad ep = 1, \ldots, N_{EP}, \quad ew = 1, \ldots, N_{EW} \tag{54}$$

3.3.5. Mass balances between ethanol warehouses and customer zones

This model adopts no stock accumulation, i.e. steady-state operation, in such way that the total amount of ethanol stored in warehouse ew has to be delivered to some customer zones, then

$$\sum_{ep=1}^{N_{EP}} Q^{eth}_{ep,ew} = \sum_{k=1}^{N_K} Q^{eth}_{ew,k} \quad ew = 1, \ldots, N_{EW} \tag{55}$$

The minimum and maximum demands must be fulfilled, so

$$\sum_{ew=1}^{N_{EW}} Q_{sw,k}^{eth} \geq Dem_{eth,k}^{LO} \quad k = 1, \ldots, N_K \tag{56}$$

$$\sum_{ew=1}^{N_{EW}} Q_{ew,k}^{eth} \leq Dem_{eth,k}^{UP} \quad k = 1, \ldots, N_K \tag{57}$$

3.3.6. Mass balances between ethanol plants and customer zones for yeast production

The yeast cannot be stored because its degradation in short time. Therefore, the yeast production is directly transferred to customer zones which have minimum and maximum demands.

$$Q_{ep}^{yeast} = \sum_{k=1}^{N_K} Q_{ep,k}^{yeast} \quad ep = 1, \ldots, N_{EP} \tag{58}$$

$$\sum_{ep=1}^{N_{EP}} Q_{ep,k}^{yeast} \geq Dem_{yeast,k}^{LO} \quad k = 1, \ldots, N_K \tag{59}$$

$$\sum_{ep=1}^{N_{EP}} Q_{ep,k}^{yeast} \leq Dem_{yeast,k}^{UP} \quad k = 1, \ldots, N_K \tag{60}$$

In order to avoid flows from not existing plants and reduce the search space, the following bound can be stated

$$Q_{ep,k}^{yeast} \leq Dem_{yeast,k}^{UP} ex_{ep} \quad ep = 1, \ldots, N_{EP}, \quad k = 1, \ldots, N_K \tag{61}$$

3.4. Objective function

The objective function is the maximization of the net profit given by the sum of the total earnings for products sales minus the total costs. The considered sale incomes are given by: sugar, exported sugar, exported electricity, ethanol, and yeast sales. The considered costs are: sugar cane supply, plant and warehouse installation, ethanol plants investment, production, and transportation costs. No penalty is imposed for sugar plant running bellow its full capacity.

The total sale income is given by:

$$IS = SP_{sugar} \sum_{sw,k} Q_{sw,k}^{sugar} + SP_{ex\_sugar} \sum_{sp} Q_{sp}^{ex\_sugar} + SP_{ex\_elec} \sum_{sp} Q_{sp}^{ex\_elec} + SP_{eth} \sum_{ew,k} Q_{ew,k}^{eth} + SP_{yeast} \sum_{ep,k} Q_{ep,k}^{yeast} \tag{62}$$

where SP_p represents the selling price for the different products p.

The installation cost, *InsC*, is a fix cost for installing ethanol factories and ethanol and sugar warehouses, therefore

$$InsC = \frac{1}{HT} \sum_{ep=1}^{N_{EP}} IC_{ep} ex_{ep} + \sum_{ew=1}^{N_{EW}} IC_{ew} we_{ew} + \sum_{sw=1}^{N_{SW}} IC_{sw} ws_{sw} \tag{63}$$

where *IC* are the annualized installation cost of each facility. The expression is divided by *HT*, the production time horizon, since all the cost terms are calculated in $\$\,h^{-1}$.

The investment cost, *InvC*, is expressed through the unit sizes of each stage of ethanol plants, therefore

$$InvC = \frac{CCF}{HT} \sum_{ep=1}^{N_{EP}} \left[\sum_{j=batch} \alpha_{j,ep} NU_{j,ep} V_{j,ep}^{\beta_{j,ep}} + \sum_{l=semicont} \alpha_{l,ep} A_l^{\beta_{l,ep}} \right] \tag{64}$$

where *V* and *A* represents the batch and semicontinuous unit sizes respectively, $NU_{j,ep}$ is the number of parallel units of batch stage *j* in plant *ep* (*NF* for fermentation and *ND* for distillation), $\alpha_{j,ep}$, $\alpha_{l,ep}$, $\beta_{j,ep}$ and $\beta_{l,ep}$ are capital cost coefficients according to Corsano et al. (2006) for units of stages *j* and *l* in plant *ep*, and *CCF* is a Capital Charge Factor, *CCF* = 0.225, that considers an amortization term of 0.1 plus 0.125 corresponding to maintenance cost. Again, the expression is divided by *HT*, in order to standardize the cost unit in $\$\,h^{-1}$.

The operation cost, *OC*, involves the raw material processed in sugar cane plants (sugar cane), inoculum and the fresh water consumption in ethanol process,

$$OC = \sum_{sp}^{N_{sp}} C_{sp}^{MC} MC_{sp} + \sum_{ep=1}^{N_{ep}} \frac{1}{CT_{ep}} (CInoc_{ep} V_{ep}^{inoc} + Cwat_{ep} Wat_{ep}) \tag{65}$$

where C_{sp}^{CM}, $CInoc_{ep}$, and $Cwat_{ep}$ represent the sugar cane, the inoculum, and the water cost coefficients respectively. The disposal cost, *DispC*, considers the residue from the centrifuge (discarded cream) and the vinasses discarded,

$$DispC = \sum_{ep=1}^{N_{ep}} \frac{1}{CT_{ep}} \left[\left(Z_e + Z_T + \frac{S_{DV,ep}}{Os} Z_{BO} \right) DVR_{ep} + Z_{cream} VR_{ep} \right] \tag{66}$$

where the coefficient for vinasses disposal are: Z_e, the reception and conveyance charge per m^3, Z_T the volumetric and primary treatment cost per m^3, *Os* the concentration of settled sewage ($kg\,m^{-3}$), and Z_{BO} the biological oxidation cost per m^3 of settled sewage. The value for *Os* is $0.2\,kg\,m^{-3}$ and the parameters Z_e, Z_T and Z_{BO} are adopted according to Bates (1981), and they are varied in the Examples in order to analyze the disposal cost influence in the SC and plant design. $S_{DV,ep}$ is the vinasses substrate concentration ($kg\,m^{-3}$), which is a optimization variable.

The centrifuge disposal cost is calculated according to the discarded volume, VR_{ep}, and Z_{cream} is the corresponding cost coefficient.

Finally, the transportation cost, *TrC*, is calculated according to the amounts of transported sugar, molasses, filter juices, ethanol and yeast.

$$TrC = \sum_{sp,sw} CTr_{sp,sw} Q_{sp,sw}^{sugar} + \sum_{sw,k} CTr_{sw,k} Q_{sw,k}^{sugar} + \sum_{sp,ep} CTr_{sp,ep}^{rw} Q_{sp,ep}^{rw} + \sum_{ep,ew} CTr_{ep,ew} Q_{ep,ew}^{eth} + \sum_{ew,k} CTr_{ew,k} Q_{ew,k}^{eth} + \sum_{ep,k} CTr_{ep,k} Q_{ep,k}^{yeast} \tag{67}$$

where $CTr_{a,b}$ are the transportation cost coefficient from *a* to *b*, and *rw* corresponds to molasses and filter juices.

Therefore, the objective function is the maximization of the net profit:

$$Max\ NP = IS - (InsC + InvC + OC + DispC + TrC) \tag{68}$$

The proposed approach is a MINLP model. The binary variables are those used for assigning the number of parallel units in ethanol plants, and those used for allocating ethanol plants, and ethanol and sugar warehouses. The non-linear constraints are presented in the ethanol plant design model, and some of them are non-convex constraints. Finally, all the SC design constraints are linear.

It is worth mentioning that all the model parameters are deterministic. However in practice, this kind of problems is affected by several variations, and uncertainty should be considered in order to reach a more realistic formulation. But, uncertainty consideration gives raise to a more complex formulation since the problem is generally tackled through different stochastic scenarios, increasing the number of decision variables and consequently the computational resolution effort. Since the proposed approach is complex due to

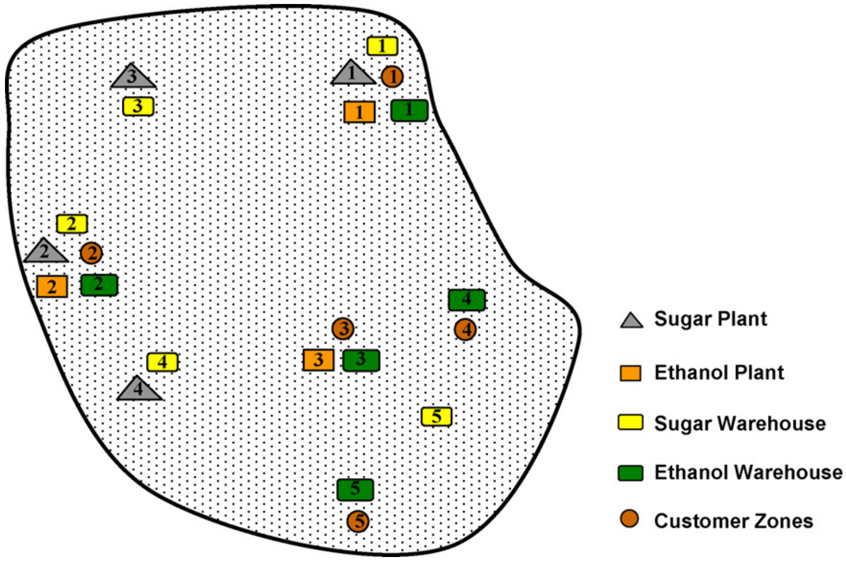

Fig. 3. SC possible node locations.

Table 2
Minimum and maximum product demands.

Customer zone	Sugar demands (ton h^{-1})		Ethanol demands (kg h^{-1})		Yeast demands (kg h^{-1})	
	Min	Max	Min	Max	Min	Max
1	0	30	1000	3000	0	2000
2	10	25	1000	3000	0	2000
3	20	40	1000	3000	0	2000
4	10	80	0	3000	0	2000
5	0	30	0	3000	0	2000

the simultaneous SC and plant optimization and the use of detailed formulation, a stochastic model will be proposed in a future work.

4. Examples

In this section different examples are presented in order to evaluate sustainable designs for a SC and ethanol plants involved in it. In each case, the model parameters regarding disposal cost for vinasses and centrifuged cream are changed in order to assess different sustainable production–distribution scenarios.

All the examples where implemented and solved in GAMS (Brooke et al., 1998) on an Intel (R) Core2, 1.86 Ghz. The model comprises 944 equations, 938 continuous variables and 35 binary variables, and the optimal solutions are found (with 0% optimality gap) in the from17 to 25 CPU seconds.

4.1. Example 1

The model is implemented for a SC considering 4 sugar plants, 5 customer zones, and up to 3 ethanol plants, 5 sugar warehouses, and 5 ethanol warehouses. The possible locations for ethanol plants and warehouses are shown in Fig. 3. The problem data does not represent a real problem but the nodes where depicted in a map for a better comprehension. The minimum and maximum demands for each product at each customer zone are depicted in Table 2. The produced sugar is transported to sugar warehouses, and then to customer zones. The corresponding transportation costs are shown in Tables 3 and 4 respectively. Molasses and filter juice transportation costs are in Table 5, while ethanol transportation cost from plants to warehouses and from warehouses to customer zones are shown on Tables 6 and 7 respectively. Finally, the yeast is directly transported to customer zones because its fast degradation. The yeast transportation cost from ethanol plants to customer zones is adopted from Table 6, due to the proximity of customer zones to ethanol warehouses.

The warehouse maximum capacity is equal to 50, 100, 80, 50, and 50 tons for sugar warehouses 1–5 respectively, while for ethanol warehouses the maximum capacities are 8000, 5000, 9000, 5000, and 5000 kg respectively. The ethanol plant capacity is handled through the bounds on its unit sizes. In this case, the inoculum preparation tank is upper bounded by 500 m^3. Since the downstream process units do not add material (no input streams exists), no bounds are established for the other process stages. Besides

Table 3
Transportation costs from sugar plant to sugar warehouses ($ h ton^{-1}).

sp	*sw*				
	1	2	3	4	5
1	0.1	5	3	20	25
2	5	0.1	5	10	8
3	3	5	0.1	15	20
4	20	10	15	0.1	12

Table 4
Transportation costs from sugar warehouses to customer zones ($ h ton^{-1}).

sw	Customer zones (*k*)				
	1	2	3	4	5
1	0.1	5	10	20	30
2	5	0.1	7	15	20
3	3	5	15	22	25
4	20	10	15	20	15
5	25	8	10	1	5

Table 5
Molasses and filter juices transportation costs ($\$ \, h \, m^{-3}$).

sp	Ethanol plant 1		Ethanol plant 2		Ethanol plant 3	
	Molasses	f. juices	Molasses	Filter juices	Molasses	Filter juices
1	0.1	0.1	5	5	10	10
2	5	5	0.1	0.1	7	7
3	3	3	5	5	15	15
4	20	20	10	10	15	15

Table 6
Transportation costs from ethanol plants to ethanol warehouses and yeast transportation costs between ethanol plants and customer zones ($\$ \, h \, kg^{-1}$).

ep	Ethanol warehouses (*ew*)				
	1	2	3	4	5
1	0.01	0.5	1	2	3
2	0.5	0.01	0.7	1.5	2
3	1	0.7	0.01	0.5	1.2

Table 7
Transportation costs from ethanol warehouses to customer zones ($\$ \, h \, kg^{-1}$).

ew	Customer zones (*k*)				
	1	2	3	4	5
1	0.01	0.5	1	2	3
2	0.5	0.01	0.7	1.5	2
3	1	0.7	0.01	0.5	1.2
4	2	1.5	0.5	0.01	1
5	3	2	1.2	1	0.01

limiting the capacity through unit sizes, the model proposes an upper bound for ethanol production given by $Q_{ep}^{UP} = \sum_{k=1}^{N_K} D_{eth,k}^{UP} = 15,000 \, kg \, h^{-1}$.

The selling price is $100\$ \, ton^{-1}$ for sugar and $1.2\$ \, kg^{-1}$ for ethanol. The yeast is not sold since is considered a residue.

The disposal cost coefficients adopted in this example are $Z_{cream} = 10\$ \, m^{-3}$, $(Z_e + Z_T) = 0.055\$ \, m^{-3}$ and $Z_{BO} = 0.0432\$ \, m^{-3}$.

In the optimal solution all ethanol plants, four sugar warehouses, and three ethanol warehouses are allocated. The SC design is shown in Fig. 4. The maximum demand of sugar for customer zones 1–3 and 5 is satisfied, while the amount of sugar delivered to customer zone 4 is $64.75 \, ton \, h^{-1}$ and no sugar is sold to external markets. The available sugar cane is processed in each sugar plant. Also, the maximum demands of ethanol of customer zones 1–4 are

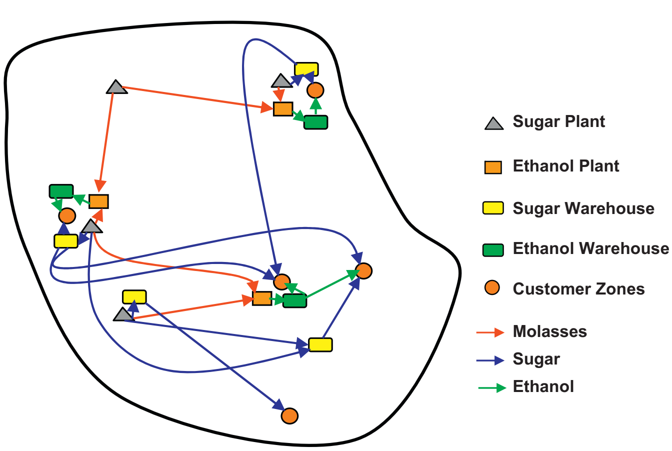

Fig. 4. Optimal SC design for Example 1.

Table 8
Economical results for presented examples.

	Example 1	Example 2	Example 3	Example 4
Income for sales				
Sugar	18,975	18,975	18,975	18,975
Ethanol	14,400	14,400	14,400	14,400
Yeast	0	0	0	3000
Electricity	270	219	227	284
Costs				
Molasses transport	241	271	241	242
Yeast transportation	0	0	1056	60
Ethanol to warehouses	120	120	120	120
Transportation				
Ethanol to customers	1590	3060	1590	1590
Transportation				
Sugar to warehouses	693	693	693	693
Transportation				
Sugar to customers	1037	1037	1037	1037
Transportation				
Sugar cane (raw mat.)	3300	3300	3300	3300
Sugar warehouses inst.	400	400	400	400
Ethanol warehouses inst.	300	200	300	300
Ethanol plant inst.	1500	1000	1500	1500
Inoculum	263	193	142	265
Investment	2345	3049	4662	2618
Vinasses disposal	48	0	0	48
Cream disposal	75	83	0	38
Total net benefit	21,733	20,188	18,561	24,448

satisfied (customer zone 5 does not receive ethanol). The electricity produced at sugar plants is enough to satisfy the ethanol plant electricity demands, and 1128.7 kWh are sold to the local power network.

Ethanol plants 1 and 2 produces $3000 \, kg \, h^{-1}$ of ethanol each one, while ethanol plant 3 produces $6000 \, kg \, h^{-1}$. The optimal plant designs are presented in Fig. 5. The optimal plant configurations for ethanol plant 1 and 2 are similar and they have two units out of phase for fermentation stage. For ethanol plant 3, three units out of phase are used in fermentation stage, while distillation is duplicated. It is worth noting that ethanol plant 3 produces a bigger amount of ethanol, and therefore bigger unit sizes are needed. Semicontinuous items of distillation stage are smallest since bigger processing time is obtained for this stage in this plant. Duplication is carried out in order to reduce the plant cycle time.

All the ethanol plants discard the centrifuge residue and the total produced vinasses. Since disposal cost for both residues is relatively small, the solution chooses to discard them.

The vinasses recycle increase the inoculation tank sizes and dilute the blend of molasses and inoculum, and therefore the substrate concentration of the inoculation. Then, long processing time at fermentation stage is needed in order to reach the specified ethanol and biomass concentration (Eqs. (14) and (15)). Moreover, the use of vinasses increases the unit sizes, and therefore the investment cost.

In this case, no yeast is produced, since yeast production involves adding two units: evaporator and dryer; and consequently the investment cost is increased. When centrifuge residual cost is low and yeast has not an attractive selling price (in this case the price is considered equal to zero), the yeast production is not profitable and therefore, the centrifuge residuals are discarded.

It is worth mentioning that, due to transportation costs, the customer zones are supplied in first place by plants that are in the same region: customer zone 1 by sugar and ethanol plant 1, customer zone 2 by sugar and ethanol plant 2, and customer zone 3 by ethanol plant 3. Then, according to product availability and transportation costs, the remainder customer zones are supplied.

The first column of Table 8 shows the economical results for this example.

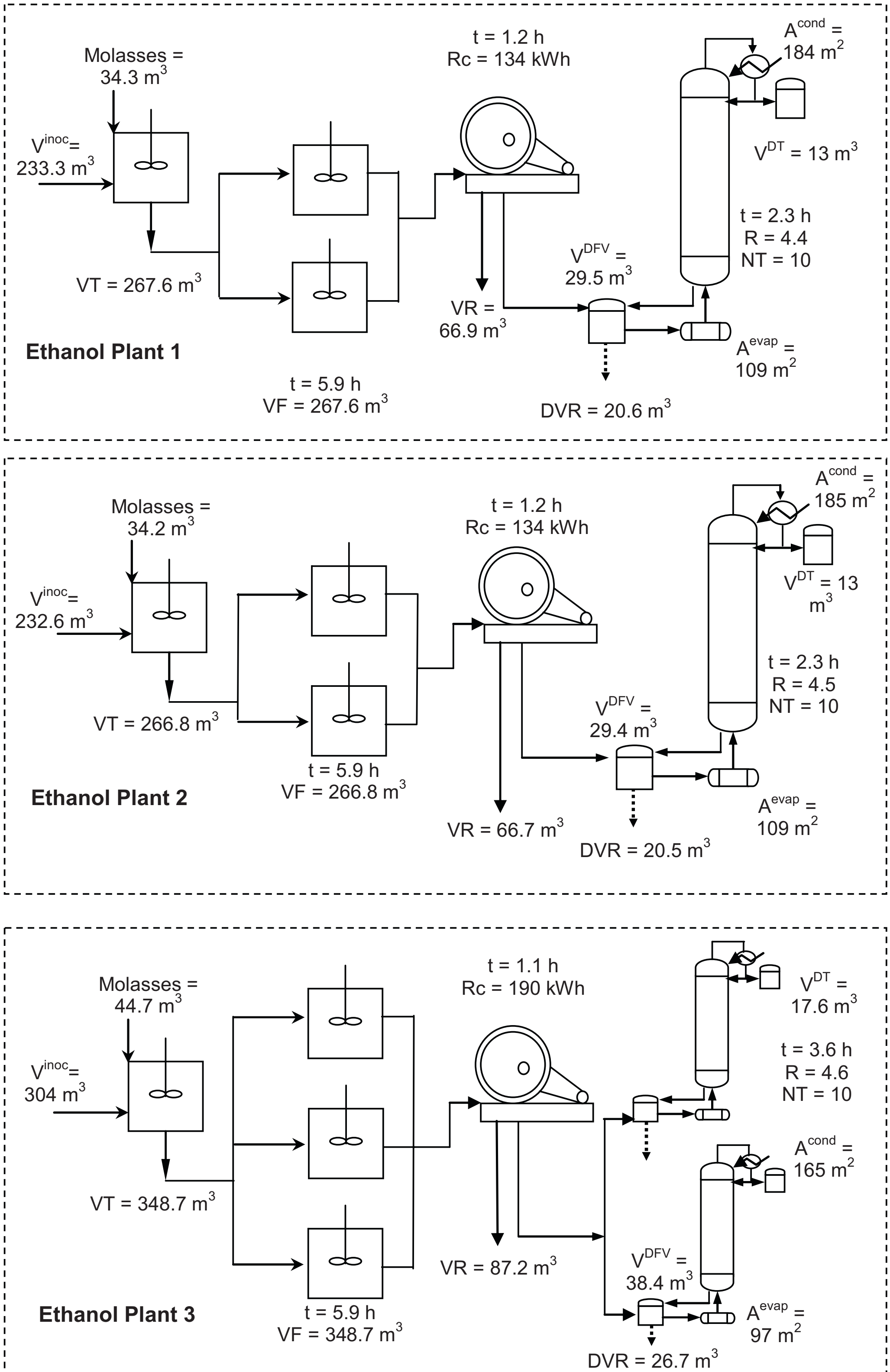

Fig. 5. Optimal design for ethanol plants of Example 1.

4.2. Example 2

In order to avoid the residue discarding, the vinasses disposal cost (Eq. (66)) is increment to $Z_e + Z_T = 5.5\,\$\,\mathrm{m}^{-3}$ and $Z_{BOC} = 4.32\,\$\,\mathrm{m}^{-3}$. All the remainder parameters are the same used in the previous example.

The optimal solution changes considerably the SC design from the preceding instance. In this case, two ethanol plants and two ethanol warehouses are allocated as it is shown in Fig. 6.

The vinasses penalization forces to recycle all the produced vinasses to inoculation tank, and therefore, the fermentation unit sizes are increased. For that reason, the solution selects only two

Table 9
Optimal design and processing times for ethanol plant for Example 2.

	inoc tank	fer	cen	dist					
				DFV	evap	R	NT	cond	DT
Unit sizes	430 m^3	430 m^3	357 kWh	140 m^3	522 m^2	13.3	12	833 m^2	19.7 m^3
Processing times (h)		7	0.7	1.9					

plants, and 6000 kg h^{-1} of ethanol is produced in each one for satisfying the maximum demands of clients 1–4. Therefore, only two ethanol warehouses are located near to the ethanol plants. In this way, the ethanol transportation cost is increased. The electricity produced at sugar plants is enough to satisfy the ethanol plant electricity demands, and 910.6 kWh are sold to the local power network.

The design of both plant are similar and it is shown in Table 9. Yeast is not produced and all the centrifuge residual is discarded (107.2 m^3 in each plant). The inoculum tank size is incremented due to the use of vinasses and the processing times in fermentation stage are longer because vinasses dilute the fermentation broth, and therefore, more time is needed to attain the convenient product concentration. Consequently, three units out of phase are used in fermentation stage. Also, more molasses are consumed (54 m^3) in each plant. The sizes for distillation stages are also incremented due to mass increase and concentration decrease.

The economical results are displayed in the second column of Table 8. It can be noted that the ethanol transportation cost is incremented (92%) as consequence of reducing the number of plants and warehouses for this production. The investment cost is also incremented (30%) due to the use of bigger unit sizes. In addition, the centrifuge residual cost is 10% bigger than the previous instance because fermentation sizes increase.

It is worth to highlight the impact of the vinasses disposal cost in the SC design. This fact is not possible to analyze when SC design and plant design are separately tried. When sustainable designs are approached, all the SC and plant process variables must be simultaneously optimized in order to assess the several tradeoffs that exist among them. The proposed formulation allows the analysis of different scenarios for a sustainable ethanol SC.

4.3. Example 3

In this example the cream disposal cost is increased to 200$ m^{-3} in order to highly penalize this disposal. All the remaining parameters are considered as Example 1.

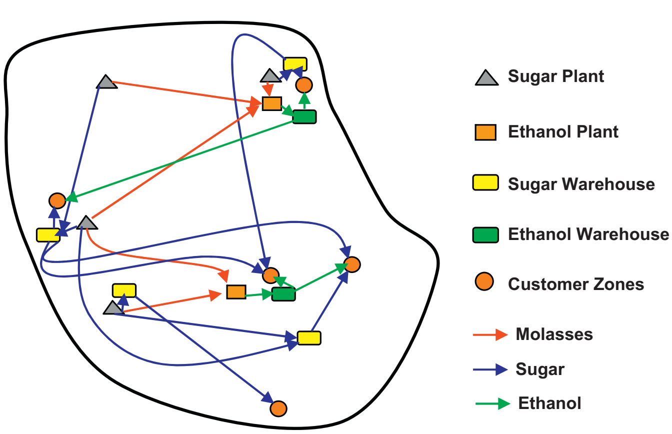

Fig. 6. Optimal SC design for Example 2.

The optimal SC design is similar to that obtained in Example 1 optimal solution (Fig. 4): four sugar warehouses, three ethanol plants and three ethanol warehouses. Also, sugar and ethanol productions and distributions are equal to Example 1. The yeast production is equal to 2000 kg h^{-1} in ethanol plant 1, and 2000 kg h^{-1} in ethanol plant 2, and 3992 kg h^{-1} in ethanol plant 3. The yeast is transported to customer zones 1 and 2 from ethanol plant 1 and 2 respectively, while the yeast produced in ethanol plant 3 is sent to customer zones 3 and 4. Customer zone 5 only receives sugar. There are 947.8 kWh of excess electricity sold to the power station.

Neither cream nor vinasses are discarded, but the net profit is 14.6% reduced, due to an increment in the investment cost and yeast transportation costs. For fermentation stage of all ethanol plants, three units out of phase are used. In order to obtain bigger biomass concentration for yeast production, longer processing times are required at this stage. Then, with the aim of reducing production cycle time, three units out of phase are selected. The design of ethanol plants 1 and 2 are similar, and unit sizes and processing times for each plant are depicted in Table 10.

The third column of Table 8 shows the economical results.

4.4. Example 4

Finally, a selling price for yeast is assigned in order to evaluate the profitability (or not) of this production. All the model parameters are considered as in Example 1 and the yeast selling price is taken equal to 0.5$ kg^{-1}.

The optimal SC design is the same obtained in Example 1 and shown in Fig. 4, except for the production of yeast, which in this instance is produced in ethanol plants 1, 2 and 3 and sent to customer zones 1, 2, and 3 respectively. It is worth noting that yeast is produced in order to satisfy the "local" demand, i.e. the demand of the customer zone located near to each ethanol plant. In other words, for the problem parameters presented in this work, the yeast production is profitable when it is sent to customers located close to production plants. Since the centrifuge disposal is not highly penalized in this example, the optimal solution discards part of the centrifuge broth and processes the necessary to satisfy the local demand. Again, the electricity produced at sugar plants is sufficient

Table 10
Optimal plant designs for Example 3.

	Ethanol plant 1 and 2		Ethanol plant 3	
	Unit sizes	Processing times (h)	Unit sizes	Processing times (h)
inoc tank	263 m^3		500 m^3	
fer	263 m^3	9.2	500 m^3	9
cen	164 kWh	0.95	350 kWh	0.84
evap	63 m^2		134.7 m^2	
dry	159 m^2		344 m^2	
Distillation		2.4		2.4
DFV	111 m^3		208 m^3	
evap	380 m^2		778 m^2	
R	19.6		20.7	
NT	13		13	
cond	642 m^2		1316 m^2	
DT	19.5 m^3		24.8 m^3	

Table 11
Optimal plant designs for Example 4.

	Ethanol plant 1 and 2		Ethanol plant 3	
	Unit sizes	Processing times (h)	Unit sizes	Processing times (h)
inoc tank	174 m^3		344 m^3	
fer	174 m^3	5.9	344 m^3	6
cen	107.8 kWh	0.95	225.7 kWh	0.9
evap	23.2 m^2		24.7 m^2	
dry	106 m^2		112.9 m^2	
Distillation		1.3		1.4
DFV	19 m^3		38 m^3	
evap	122 m^2		246 m^2	
R	4.3		4.6	
NT	10		10	
cond	206 m^2		417 m^2	
DT	8.6 m^3		17.4 m^3	

to satisfy the ethanol plant electricity demands, and 1182.6 kWh are sold to the local power network.

The optimal ethanol plant configuration is the same for all plants: three units out of phase are used for fermentation stage, while distillation is not duplicated. Ethanol plants 1 and 2 have similar designs, and the unit sizes and processing times are shown in Table 11.

Since vinasses disposal is not hardly penalized they are not recycled and therefore, the inoculum tank size is smaller and the inoculum broth is more concentrated than the one obtained in Example 3. In this way, all the process operations are more efficient, yeast is produced and sold, and investment cost is not excessively incremented comparing with Example 1 solution.

The total benefit is 11% increased in this solution due to the income for yeast sales. The last column of Table 8 shows the economical results for this example.

4.5. General remarks

The analysis made to the previous examples shows that the extraction of filter juices is not convenient because it decreases sugar and molasses productions. In all cases, since sugar production/distribution is profitable, the total available amount of sugar cane is processed in all the sugar plants. Therefore, the maximum amount of sugar and molasses is produced in each plant for supplying almost all the maximum sugar demands (except customer zone 4), and molasses requirements for producing ethanol.

The produced electricity in each sugar plant is enough to cover the electricity demand for all the ethanol plants allocated, and the remaining electricity is sold to the local power station and the income for this sale is shown in Table 8.

In order to reduce cream disposal, the best alternative will be supply yeast to customers near to the ethanol plants. From Examples 3 and 4, it can be concluded that better solution can be reached if no upper bounds are imposed for yeast demands, such that all the produced yeast can be consumed in the nearest zone.

As can be observed from the examples, customer zone 5 is far-off the ethanol plants/warehouses, and therefore the ethanol supply to this customer is not profitable.

5. Conclusions

In this work, a MINLP model for the simultaneous optimization of SC and plant design for producing ethanol from sugar cane was proposed. The model embeds a detailed formulation for the ethanol plants considered in the SC. Residual recycle and derivative production are assessed in order to attain sustainable designs.

The approach represents a tool for analyzing different production–distribution systems according to the environmental impact parameters adopted in the mathematical formulation. This work was focused on sustainable SC and process designs, for that reason the analysis was made over the disposal cost parameters. But the approach also serves as a tool for evaluating different scenarios considering fluctuations in cost, demands, raw material supply, etc. Through the proposed examples, it can be highlighted that the more profitable solution is when three ethanol plants and warehouses are installed. But, when vinasses are recycled to inoculation tank, the units sizes are increased and the blend is diluted. Then, longer fermentation times are needed in order to reach convenient concentrations. Consequently, in order to reduce the cycle time, more units out of phase are used, incrementing the investment cost. Therefore, two ethanol plants are used instead of three, and a different design for the SC is obtained.

When the centrifuge residue disposal is penalized, this residue is totally processed to produce yeast. In this case, the SC considers 3 ethanol plants and warehouses but the plant performances are different that those obtained when yeast is not produced. More fermentation units are needed with longer processing times in order to obtain bigger biomass concentrations for yeast production. Therefore, the investment cost is increased and the total net profit is decreased.

The simultaneous optimization allows the evaluation of several compromising situations between the sugar and ethanol processes and its design variables. The model proposed in this article lets the evaluation of the effects on the SC design, due to the inclusion of a detailed formulation of the ethanol plant. In fact, in the discussion of the results obtained, it was shown how equipments sizes, investment and transportation cost, environmental impact of ethanol by-products change according to the variation of the processes variables. This is the aggregated value of this approach.

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