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Research Article

Incorporation of Mass and Energy Integration in the Optimal Bioethanol Separation Process

A techno-economic analysis for the separation process in bioethanol production is presented. Optimized azeotropic separation processes in conjunction with process integration (mass and energy) are considered to simultaneously enhance the results from economic and environmental points of view. Process integration improves significantly the separation process because it helps to reduce the overall energy required in the reboilers based on energy integration and additionally to diminish the amount of required solvent based on mass integration. The SYNHEAT optimization model was applied for energy integration whereas a direct recycle strategy was implemented for the mass integration process. The best separation processes obtained correspond to an integrated conventional separation sequence with energy integration to ethanol-water mixture III and integrated optional separation sequences with energy integration to ethanol-water mixture III, with significant savings in utility costs and possible recycling of nearly all solvent.

Keywords: Bioethanol separation, Energy integration, Mass integration, Process integration

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1 Introduction

Conversion of abundant lignocellulosic biomass to biofuels as transportation fuels represents a viable option for improving energy security and reducing greenhouse gas emissions because of the photosynthetic sequestration of carbon dioxide by the biomass during plant growth [1]. Unlike fossil fuels, which derive from plants that grew millions of years ago, biofuels are produced from plants growing today. It has been reported that cellulosic ethanol and ethanol produced from other biomass resources have the potential to cut greenhouse gas emissions by 86 % [2]. Bioethanol production has become one of the most studied processes in the last two decades because of the necessity of finding alternative renewable fuels.

Bioethanol production at industrial scale relies on several processes, such as corn-to ethanol, sugarcane-to-ethanol, and basic and integrated lignocellulosic biomass-to-ethanol [3]. Basically, the raw materials undergo some pretreatment steps and then enter the fermentation stage where bioethanol is produced. A common feature of all bioethanol technologies is the production of diluted bioethanol in the range of 5–12 wt % ethanol that needs to be further concentrated [4]. According to the current international bioethanol standards, the maximum allowed water content is 0.2 vol % (EN 15376, Europe), 0.4 vol % (ANP no. 36/2005, Brazil) or 1.0 vol % (ASTM D 4806, USA) [5]. Purification of bioethanol fuel requires energy in the distillation steps to concentrate the diluted streams from the fermentation step and to overcome the azeotropic behavior of the ethanol-water mixture. The conventional separation sequence consists of three distillation columns performing several tasks with high energy penalties: preconcentration of ethanol, extractive distillation, and solvent recovery. Despite the novel recent developments in pervaporation and adsorption with molecular sieves, the industrial production of anhydrous bioethanol is still dominated by extractive distillation as separation method [5].

The first step is typically carried out in a preconcentration distillation column that concentrates bioethanol from 5–12 wt % up to 92.4–94 wt %. The second step involves ethanol dehydration up to higher concentrations above the azeotropic composition, hence it is more complex and of greater interest. Several alternatives are available and well-described in the literature: pervaporation, adsorption, pressure-swing distillation, extractive distillation, azeotropic distillation, as well as hybrid methods combining these options [5, 6].

Recently, Lasich et al. [7] reported the use of *n*-dodecane as a solvent to extract light alcohols such as ethanol and 2-propa-

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nol from water by liquid-liquid extraction. However, liquid-liquid extraction alone is unable to produce the purity levels required for bioethanol. Aviléz-Martínez et al. [8] and Vázquez-Ojeda et al. [9] proposed the design and optimization using stochastic strategies (differential evolution) of hybrid systems of liquid-liquid extraction and extractive distillation to reduce energy consumption and total annual costs for the purification step in the bioethanol production process. The liquid-liquid extraction is performed with *n*-dodecane as entrainer, reducing the concentration of water; in a second separation stage, extractive distillation is applied to reach the desired ethanol purity with glycerol as entrainer. However, all previous approaches focused on analysis and optimization of the separation system without considering process integration techniques. Process integration is a holistic approach in order to decrease the energy and raw material consumption through recycling, reusing, and regenerating process streams [10]. Furthermore, process simplification and intensification can be carried out as described by Gopalakrishnan et al. [11]. In the case of energy integration, the heat available on the process, i.e., heat excess, can be used as heating source to decrease the external energy consumption whereas for the case of mass integration, the used mass streams can be employed with an adequate treatment to reduce the external mass consumption.

The idea of process integration is to reduce as much as possible the external mass and energy consumption reusing the available mass and energy of the process (see El-Halwagi [10]). In the bioethanol separation process, the major contribution to the related cost is the external consumption of heating to run the reboilers associated to the distillation columns where usually low-pressure steam is employed which comes for the combustion of fossil fuels. However, in the distillations columns also there is cooling required for several streams in the condensers, usually by means of cooling water. In the particular case of azeotropic distillation, additionally the solvent has to be cooled down before recycling. Therefore, the separation process has several streams that need to be heated and others that require cooling. Consequently, the application of energy integration techniques, particularly the use of heat exchanger networks (HEN) approaches, can be attractive to integrate energetically the process. This way, several methodologies have been reported for the optimal synthesis of HEN. For comprehensive reviews see the papers in [12–17]. In this context, the SYNHEAT optimization formulation proposed by Yee and Grossmann [18] is a promising approach for cost-optimal synthesis of HEN accounting for the energy and capital costs simultaneously. This method has been widely used as a basis for HEN synthesis; see, e.g., [19–28] because it is very easy to implement and able to solve moderate-scale HEN problems.

In the bioethanol separation process, the addition of a solvent to separate the azeotrope is required which can mean considerable costs. Therefore, this solvent can be recovered and recycled to the process in order to reduce the fresh solvent consumption. This recycling process may offer both economic and environmental benefits. To solve the optimal mass integration problem, several approaches for the synthesis of recycle/reuse/regeneration networks have been proposed [10, 11, 29–31]. The sinks-sources representation is particularly useful for mass integration in the process industry where process streams are identified that can be recycled and processes that require specific streams. The problem can be solved for a direct recycle configuration, e.g., [32–34], and including regeneration processes [32, 35, 36].

The integration approaches enable significant reductions in the use of external mass and energy. Since these are the major contributions in the associated costs of the separation process, it is attractive to include these techniques in the optimal synthesis of an integrated separation process for bioethanol production. In this context, a techno-economic analysis for the bioethanol separation process is presented, including evaluation and optimization of several separation configurations and simultaneously accounting for mass and energy integration to reduce the overall cost.

2 Optimization Methodology

In a first step, optimization for the separation sequence is carried out, based on the approach by Vázquez-Ojeda et al. [9] which incorporates design and optimization for the dehydration process of bioethanol considering two separation sequences: a conventional arrangement and an alternative arrangement based on liquid-liquid extraction. A differential evolution algorithm with restrictions coupled to the process simulator Aspen Plus^{TM} as optimization methodology was used. This optimization for the separation sequence provides the configuration that minimizes the utility requirements (hot and cold) as well as the flow rates and temperatures for the involved streams. From these results, the streams are identified which have to be heated and cooled, their target temperatures as well as the physical properties (the mean value is taken for this purpose). Also, these results provide information about the solvent requirements as well as the sources for solvent that can be incorporated to the mass integration process. Then, the optimization formulation for the heat exchanger network is based on a stage-wise superstructure.

From the optimization for the distillation sequence, the flow rates, temperatures, and physical properties for the streams are obtained that need heating and cooling. These streams are then incorporated into the superstructure, where the hot process streams flow from the left to the right and the cold process streams from the right to the left. Then the superstructure is divided into stages where the number of stages corresponds to the maximum number of hot or cold process streams, and in each stage the heat exchange is allowed between any pair of hot and cold process streams. The existence for the exchangers is optimized through binary variables, and the hot utilities are only allowed at the left-hand side from the superstructure, whereas the use of cold utilities is only permitted at the right-hand side of the superstructure. It should be noted that the temperatures for the process streams through the superstructure are optimization variables (continuous variables) and only a limit for the temperature difference for any match in the superstructure is imposed, i.e., 5 K. This limit is just a feasibility constraint, but this does not fix the recovered heat. In this way, the SYNHEAT model simultaneously optimizes the capital and utility costs associated to the HEN. The SYNHEAT model includes overall energy balances for the involved process

streams, energy balances for each stream in each stage of the superstructure to determine the intermediate temperatures, energy balances for the hot and cold utilities, temperature differences constraints, feasibility constraints, and logical relationships to determine the existence of the heat transfer units. Finally, the objective function includes the capital costs for the heat transfer units as well as the hot and cold utility costs. This model is formulated as mixed integer nonlinear programming optimization problem and this was solved using the GAMS software.

To deal with the phase transitions in the exchangers, the sensible and latent heats are grouped and then a mean heat capacity flow rate is determined. Furthermore, the film heat transfer coefficients for the streams that exchange simultaneously latent and sensible heat are considered as pondered values for the respective type of heat. This type of formulation for manipulating the latent and sensible heat has been reported previously by Ponce-Ortega et al. [20]. The mean value for the properties of the streams was considered, i.e., the mean for the upper and lower temperatures for each stream. For additional details about this model refer to [18]. The SYNHEAT approach is applied in this paper for energy integration in the bioethanol separation process.

In this paper, for the solvent recovery process, a direct recycle representation was implemented [32], i.e., from the separation optimization process waste solvent streams are determined that can be recycled, and also the units that require solvent. With this information, a superstructure is proposed where the direct recycle of any waste solvent stream to any unit is allowed. Additionally, satisfying the solvent requirement for each unit fresh solvent is possible. This direct recycle formulation includes mass and component constraints for sources and sinks, and the model must determine the configuration that minimizes the total fresh solvent cost, i.e., the model formulation determines the flow rates between sources and sinks at the minimum cost for the fresh solvent. It should be noted that this direct recycle configuration represents a very cheap option because this does not incorporate regeneration units. A representation that contains regeneration units may increase the amount of recovered solvent but it leads to additional investment. In this paper, this direct recycle formulation for solvent recovery in the azeotropic bioethanol distillation is implemented.

One of the main limitations of the optimization process is that the implemented approach is sequential which means that first the optimization for the separating process is carried out, then the energy integration is involved, and finally the mass integration. An important improvement would be the simultaneous optimization for the system. Another essential limitation is the calculation of the stream properties. In this way, a better estimation procedure must be included to simultaneously consider the temperature dependence as well as to include the phase change effects. Furthermore, the improved mass integration process which comprises regeneration units must be included in the model to improve the solvent recovering process.

3 Case Study

Four feeds were considered modifying the molar composition ethanol/water (see Tab. 1) with a feed flow of 45.35 kmol h^{-1}; thus, for each sequence, four sequences were optimized for each of the feeds studied. Fig. 1 shows schematically the optimization methodology for conventional separation sequence (CSS). The same procedure was carried out to optimize the optional separation sequence.

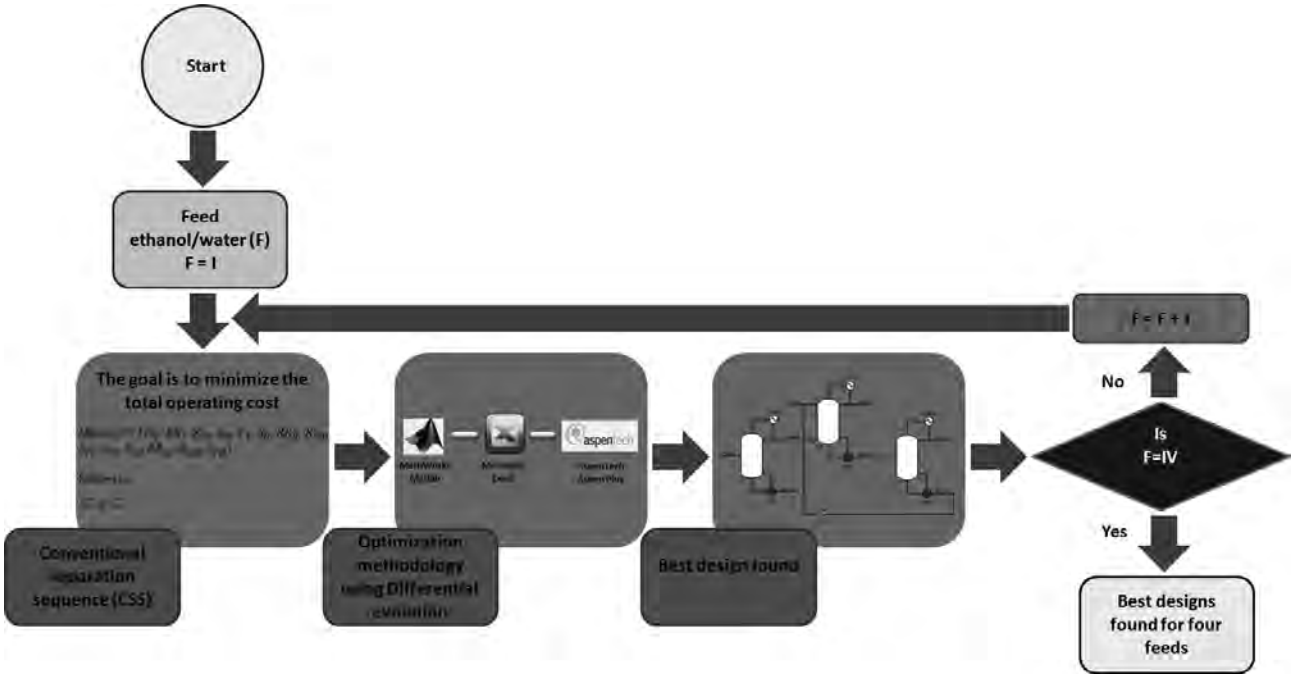

Figure 1. Flow chart of optimization methodology for conventional separation sequence (CSS).

Table 1. Feeds of ethanol-water mixture (FEEDI).

Feed flow [kmol h^{-1}]	FI	FII	FIII	FIV
Ethanol	6.80	4.54	2.27	0.91
Water	38.56	40.82	43.09	44.45
Mass composition [%]:				
Ethanol	31	22	12	5
Water	69	78	88	95

Fig. 2 illustrates the conventional separation sequence where I to IV indicate the feed corresponding to the ethanol-water mixture. Similarly, Fig. 3 presents optional separation sequences (OSS). Both figures provide detailed information on optimization results for conventional and optional separation sequences, specifying the temperatures at the inlet and outlet of condensers and reboilers. More details about the optimization of the base cases are described in Vázquez-Ojeda et al. [9]. Auxiliary units (AE) are fed with a stream of cooling water entering at 15 °C and leaving at 16 °C. Auxiliary equipment is employed to cool the bottom streams of column CIII, containing extractive distillation agent (ethylene glycol) recycled to the extractive distillation column (CII). Traces of solvent and water are removed from the top of column CIII. All condensers are fed with cooling water entering at 15 °C and leaving at 16 °C while the reboilers use steam of 450 °C.

The designs previously optimized (CSS and OSS) were retaken for applying mass and energy integration using the SYNHEAT optimization model and a direct recycle for the integration process.

4 Results

Process streams are identified from the flow sheet to conduct an energy integration process and then for a mass integration process considering the model SYNHEAT and a direct recycle configuration, respectively. Fig. 4 demonstrates the conventional separation sequence with energy integration (CSS-EI) where I to IV indicate the feed corresponding to the ethanol-water mixture.

Fig. 5 illustrates the optional separation sequence with energy integration (OSS-EI) where I to IV indicate the corresponding feed. Figs. 4 and 5 contain detailed information on optimization results for conventional and optional separation sequences with energy integration, specifying the temperatures at the inlet and outlet of the exchanger, heat duty, and the area required on this equipment.

Tab. 2 summarizes the energy consumptions for the conventional separation sequences with and without energy integration. A reduction in the consumption of utilities in the con-

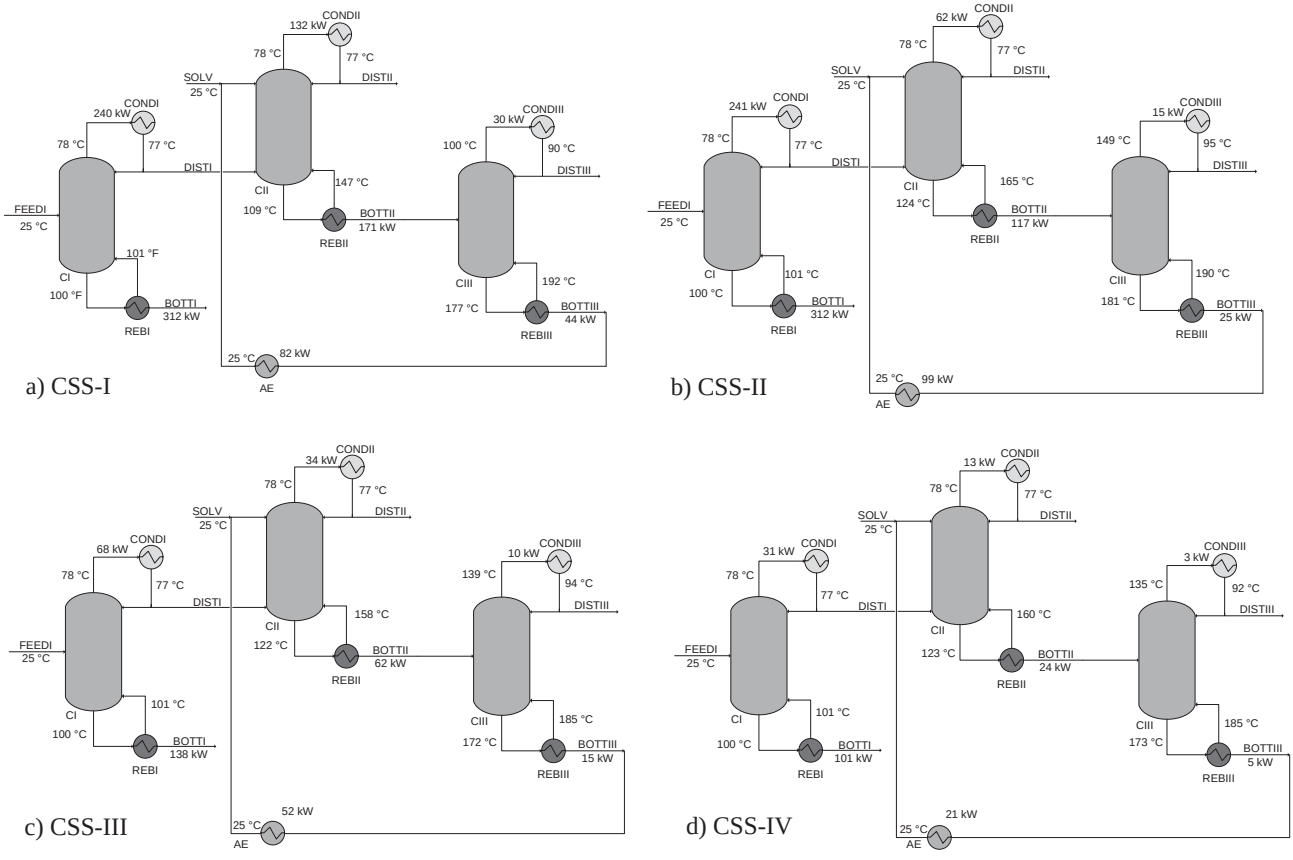

Figure 2. Conventional separation sequences based on distillation columns for purification of bioethanol (CSS).

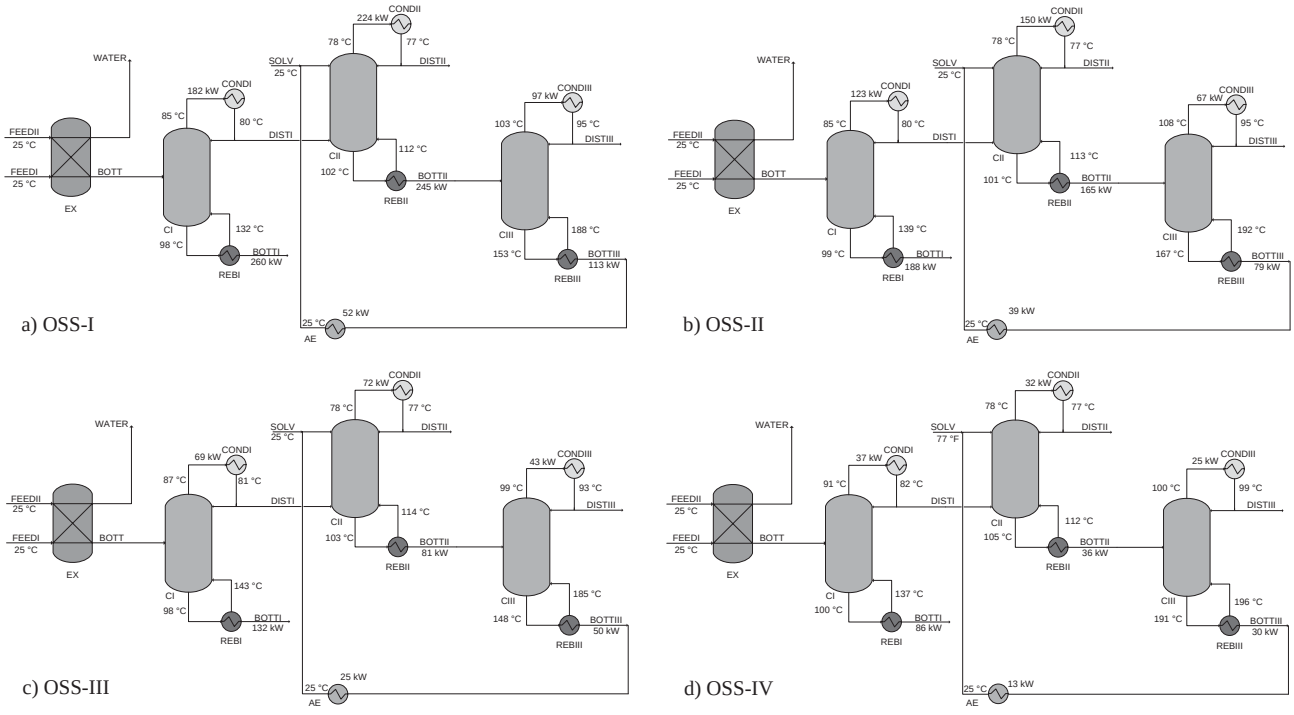

Figure 3. Hybrid configuration based on liquid-liquid extraction and extractive distillation for purification of bioethanol (OSS).

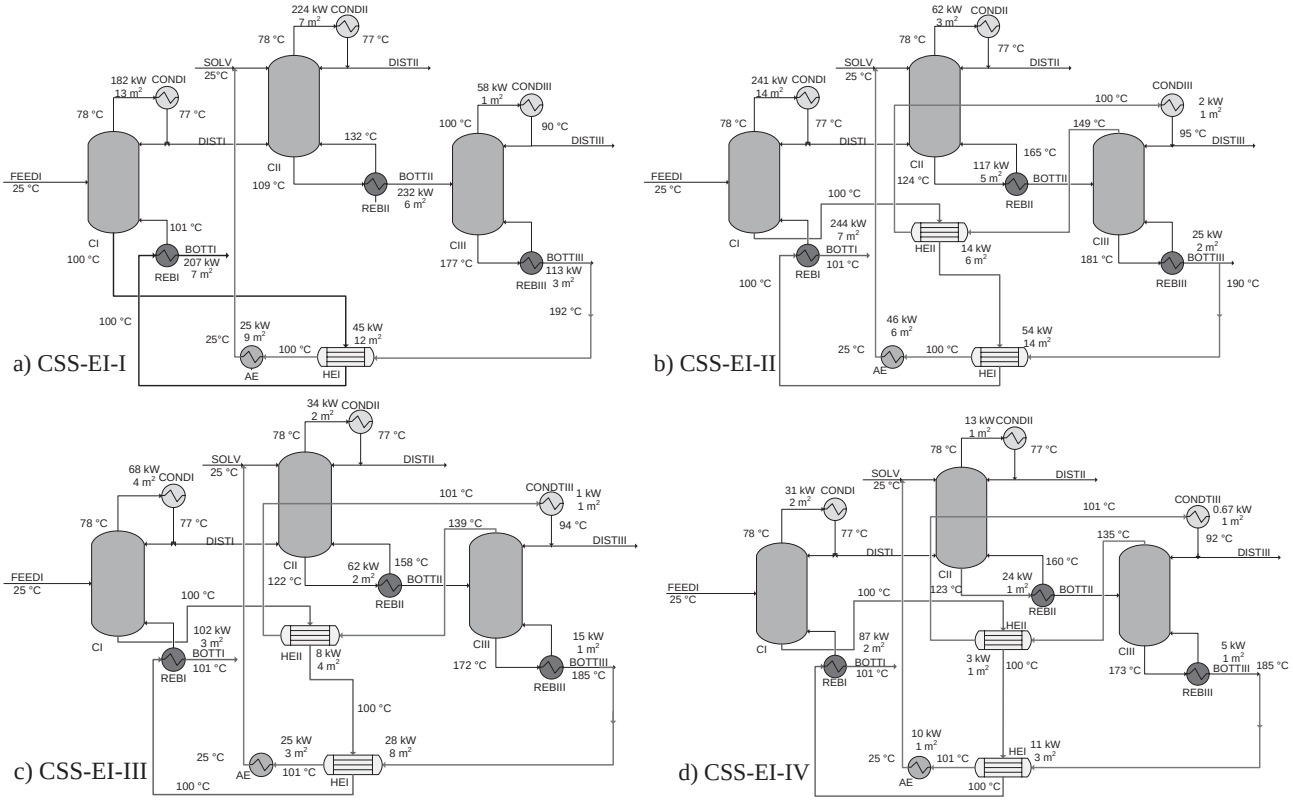

Figure 4. Conventional separation sequence for purification of bioethanol with mass and energy integration (CSS-EI).

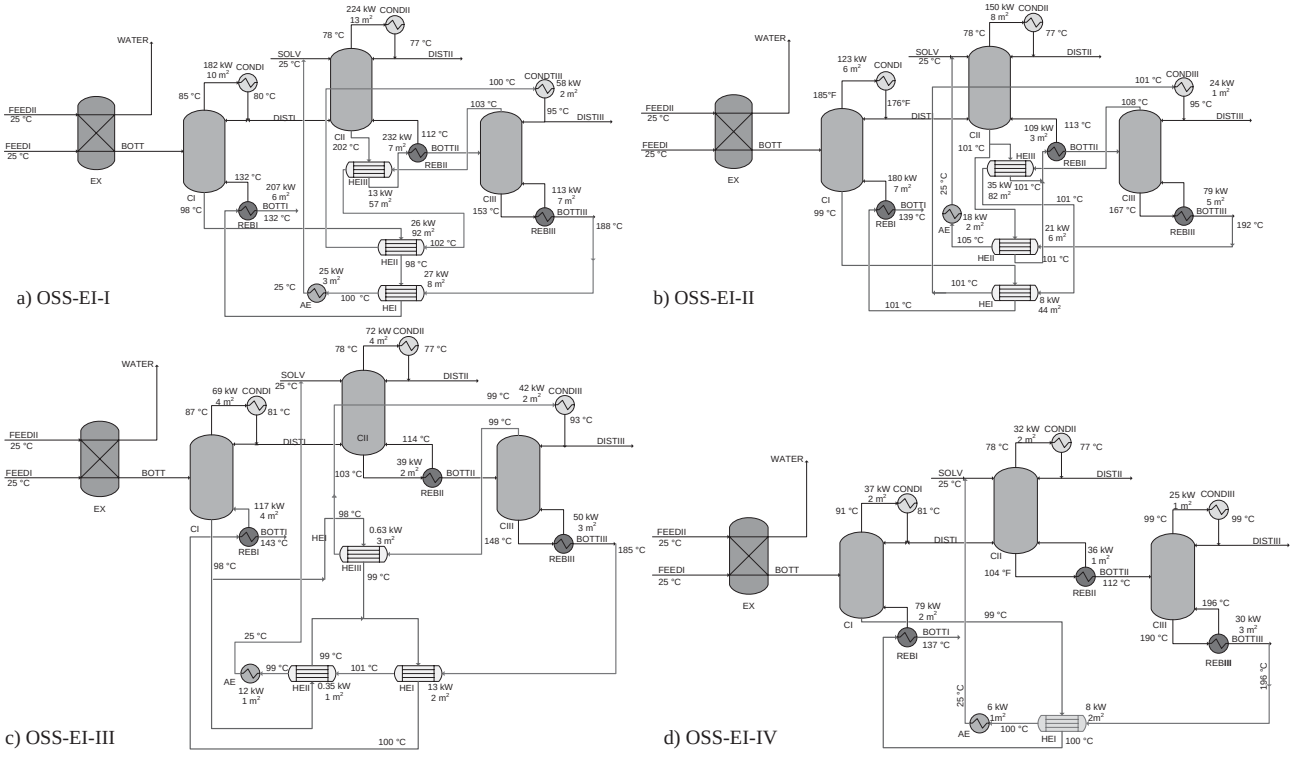

Figure 5. Hybrid configuration based on liquid-liquid extraction and extractive distillation for purification of bioethanol with mass and energy integration (OSS-EI).

Table 2. Energy requirements for the conventional separation sequences with and without energy integration.

CSS	FI			FII			FIII			FIV		
Utilities	CI	CII	CIII	CI	CII	CIII	CI	CII	CIII	CI	CII	CIII
Reboiler duty [kW]	312	171	44	312	117	25	138	62	15	101	24	5
Condenser duty [kW]	–240	–132	–30	–241	–62	–15	–68	–34	–10	–31	–13	–3
Auxiliary equipment [kW]	82			99			52			21		
CSS-EI												
Reboiler duty [kW]	267	171	44	244	117	25	102	62	15	87	24	5
Condenser duty [kW]	–240	–132	–30	–241	–62	–2	–68	–34	–1	–31	–13	–0.67
Auxiliary equipment [kW]	37			45			25			10		
Savings [%]												
Reboiler duty	8.47			14.89			16.62			10.58		
Condenser duty	0			4.34			9.85			5.92		
Auxiliary equipment	54.52			54.19			52.76			52.77		

ventional separation sequence with energy integration average of 12.64 % in the reboiler, 5.02 % in the condenser, and a reduction in energy consumption of 53.56 % for the auxiliary equipment should be noticed. CSS-EI-III provides the best savings with 16.62 % energy consumption in the reboiler, 9.85 % in the condenser, and 52.76 % in the auxiliary equipment.

Similar results are obtained in the case of optional separation sequences. Tab. 3 indicates the energy requirements for the optional separation sequences with and without energy integration. A reduction in the consumption of external utilities in the conventional separation sequence with energy integration average of 8.99 % in the reboiler, 5.18 % in the condenser, and a reduction in energy consumption of 54.18 % for the

Table 3. Energy requirements for the optional separation sequences with and without energy integration.

OSS	FI			FII			FIII			FIV		
Utilities	CI	CII	CIII	CI	CII	CIII	CI	CII	CIII	CI	CII	CIII
Reboiler duty [kW]	260	245	113	188	165	79	132	81	50	86	36	30
Condenser duty [kW]	–182	–224	–97	–123	–150	–67	–69	–72	–43	–37	–32	–25
Auxiliary equipment [kW]	52			39			25			13		
OSS-EI												
Reboiler duty [kW]	207	232	113	180	109	79	117	81	50	79	36	30
Condenser duty [kW]	–182	–224	–58	–123	–150	–24	–69	–72	–42	–37	–32	–25
Auxiliary equipment [kW]	25			18			12			6		
Savings [%]												
Reboiler duty	10.76			14.83			5.44			4.96		
Condenser duty	7.74			12.62			0.35			0		
Auxiliary equipment	52.56			54.33			53.82			56.03		

auxiliary equipment is achieved. OSS-EI-II enables the best savings with 14.83 % less consumption in the reboiler, 12.62 % in the condenser, and 54.33 % in the auxiliary equipment.

Utility costs, i.e., the cost of steam plus the cooling water of the sequence, are determined based on the method of Guthrie presented by Turton et al. [37] for the cases without and with energy integration for the different sequences studied. Tab. 4 lists the utility costs with and without energy integration. CSS-EI presents an average saving of 12.73 % and OSS-EI of 9.04 % in comparison with their respective optimized sequences without energy integration. The best results are obtained with the systems CSS-EI-III with a saving of 16.75 % (8 772 $/year) and OSS-EI-II with 14.89 % (15 710 $/year).

Tab. 5 indicates the key performance indicators with and without energy integration. CSS-EI presents an average saving to 12.66 % and OSS-EI of 8.94 % in comparison with their respective optimized sequences without energy integration. The energy requirement for the production of a ton of bioethanol is favored when considering the proposed energetic integration model which could directly benefit the product price.

Tab. 6 presents the area for all exchangers required in each one of the separation sequences. There is a considerable increment in the unit areas, however, all sequences provide savings in the utility cost (5.00 % minimum) exhibiting economic and environmental advantages. However, these results highlight the importance to consider the heat transfer units before making a decision.

In addition, mass integration is realized through direct recycling. Tab. 7 indicates the flow of ethylene glycol that is re-

Table 4. Utility costs with and without energy integration.

Utility costs [k$/year]	CSS-I	CSS-II	CSS-III	CSS-IV	OSS-I	OSS-II	OSS-III	OSS-IV
Original	129	111	52	31	151	106	64	37
	CSS-EI-I	CSS- EI-II	CSS- EI-III	CSS- EI-IV	OSS- EI-I	OSS- EI-II	OSS- EI-III	OSS- EI-IV
Energy integration	118	95	44	28	135	90	61	35
Savings [%]	8.49	14.93	16.75	10.74	10.79	14.89	5.88	5.00

Table 5. Key performance indicator with and without energy integration.

Energy requirements [kWh t^{-1} ethanol]	CSS-I	CSS-II	CSS-III	CSS-IV	OSS-I	OSS-II	OSS-III	OSS-IV
Original	1700	2205	2093	3171	1981	2084	2549	3707
	CSS-EI-I	CSS- EI-II	CSS- EI-III	CSS- EI-IV	OSS- EI-I	OSS- EI-II	OSS- EI-III	OSS- EI-IV
Energy integration	1555	1883	1742	2829	1767	1779	2403	3536
Savings [%]	8.54	14.57	16.74	10.77	10.84	14.62	5.70	4.61

Table 6. Heat exchanger areas for the separation sequences with and without energy integration.

Separation sequences	Area [m^2]			
Original	I	II	III	IV
CSS	45	37	17	8
OSS	51	36	20	12
Energy integration				
CSS-EI	54	53	26	12
OSS-EI	203	164	25	13
	Increased area [%]			
CSS-EI	20	43	53	50
OSS-EI	298	356	35	8

cycled in each of the systems and the flow of fresh solvent fed. On average, 97 % of the solvent is recycled, thus minimizing the amount of fresh solvent.

In general, conventional separation sequences are favored over optional sequences because the stream exiting the second stage of the column (CIII) before entering the condenser (CONDIII) has a higher temperature than the same stream of the optional sequence, thereby allowing greater heat transfer and consequently less transfer area. This fact becomes evident when the optional sequences are analyzed, e.g., for the sequences OSS-EI-I and OSS-EI-II more energy is integrated resulting in savings over the sequences OSS-EI-III and OSS-EI-IV but increasing significantly the area required to carry out the exchange.

5 Conclusions

A techno-economic analysis for the separation process in bioethanol production incorporating mass and energy integration is presented. Optimized integrated configurations for this azeotropic process are analyzed. Energy integration significantly helps to reduce the overall separation-associated costs, and, in addition, mass integration aids in decreasing considerably the solvent requirement. In this regard, process integration improves economically and environmentally the bioethanol separation process. Finally, the results obtained indicate that the best bioethanol separation process option considering utility cost savings, energy requirement savings, and increased area of the sequences with mass and energy integration corresponds to the conventional sequence CSS-EI-III with savings of 16.75 % in utility costs and 96 % of mass integration of solvent, and to the optional sequence OSS-EI-III with savings of 5.48 % in utility costs due to energy integration and mass integration of 97 % solvent. In this study case, conventional sequences are favored by energy integration in order to obtain substantial savings in utility costs and energy requirements with a less significant increase in area.

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Table 7. Mass integration in separation sequences with energy integration.

Mass integration	CSS-EI-I	CSS- EI-II	CSS- EI-III	CSS- EI-IV	OSS- EI-I	OSS- EI-II	OSS- EI-III	OSS- EI-IV
Ethylene glycol recycle [kmol h^{-1}] (BOTTIII)	6.80	8.30	4.50	1.79	4.42	3.21	2.18	1.09
Make-up ethylene glycol [kmol h^{-1}] (SOLV)	0.10	0.28	0.20	0.07	0.13	0.08	0.07	$1.54e^{-03}$
% Recycle	98.62	96.72	95.75	96.11	97.21	97.52	96.97	99.86

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