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Impact of the control properties on the energetic and economic performance of Heat-Integrated Distillation Columns under variable feed composition

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ABSTRACT

Heat Integrated Distillation Columns (HIDiC) are highly energy-efficient technologies whose performance has been validated through robust optimization algorithms and practical tests. Despite these configurations are dynamically controllable technologies, the simultaneous relationship between dynamics and optimal energetic and economic performance under variable feed composition has not been analyzed. Thus, this paper tackles this gap in literature. Five binary mixtures and three feed composition were examined in this study. The optimization of these configurations was firstly achieved using a Boltzmann-based optimizer while the control properties were obtained through the closed-loop process analysis using the IAE criterion and rigorous simulations in Aspen Dynamics in a second stage. Results showed that the HIDiC configurations with the best dynamic behavior do not match with the HIDiC columns with the best energetic and economic performance. However, suboptimal HIDiC configurations experienced only slightly less energetic and economic benefits but better dynamic properties that the best HIDiC configurations. Particularly, the best suboptimal HIDiC columns to separate the mixtures with relative volatility (α) lower than 1.4 were determined for a feed composition of 25 mol% for the light component. Nevertheless, the most adequate HIDiC columns to separate mixtures with $\alpha > 1.4$ were obtained for equimolar feed composition and feed composition of 75% for the light component.

1. Introduction

Sustainability for development is the current issue tracked by the international community. Each production sector is making its corresponding effort to generate products using less fresh resources (mass and energy). Since the chemical industry perspective, the improvements are tracked through the process integration. That is, instead releasing the mass and energy from the process to the environment, they are reintroduced in the same or in other processes to minimize the feed of fresh resources. Particularly, in energy terms, a high effort is focused on the purification units, such as distillation columns, as a consequence of their low capability to harness the thermal energy in an efficient way (De Koeijer & Kjelstrup, 2000; Humphrey, Seibert, & Koort, 1991). Fortunately, the search for novel distillation technologies has led to generate configurations able to cut down the energy demands (up 70%), such as the heat integrated distillation columns (Kiss & Olujić, 2014).

The elemental HIDiC configuration for purifying the dome (D) and bottoms (B) products of a binary mixture is depicted in Fig. 1.

Notice that the heat integration is performed from the rectifying section (RS), high Pressure (P_{RS}), to the stripping section (SS), low pressure (P_{SS}), by regulating the pressure using the compressor (C) and the throttling valve (TV). The compression ratio (CR) is the most important operation variable of these configurations. In this case, CR is defined by the ratio of pressures (P_{RS}/ P_{SS}) and P_{SS} is defined as 1 atm.

HIDiC configurations have obtained a large recognizing among the current intensified distillation columns due to that their best performance is found for difficult separations, such as close-boiling mixtures (Gutiérrez-Guerra et al., 2016). The separation of these kinds of systems conducts to high energy consumption and capital investment required when the separation is made using traditional columns. These improvements are produced because the heat transfer performed in the HIDiC column is distributed along the stages of the columns, in comparison with the conventional column, which receives the complete supply of energy in

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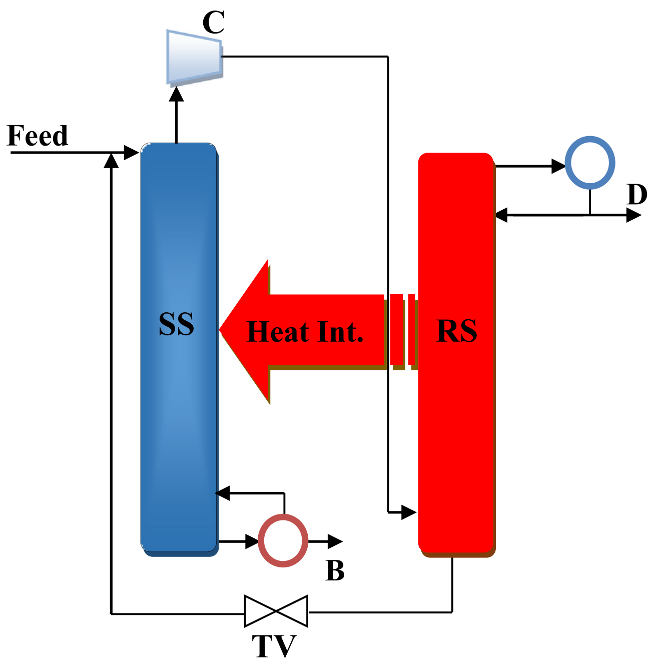


Fig. 1. Structural configuration of the HIDiC column.

the reboiler and release it through the condenser (Kiss & Olujić, 2014).

Due to their high performance, HIDiC columns have been extended to deal with reactive systems. For instance, for the synthesis of the tertiary-amyl methyl ether produced energy savings of 22% in relation to the traditional reactive column (Vanaki & Eslamloueyan, 2012). Similarly, important reductions (30% and 40%) of total annual cost (TAC) were obtained by comparing a reactive HIDiC configuration with the reactive pervaporation and pressure-swing distillation (PSD) processes (Babaie & Nasr Esfahany, 2020). Again, the production of tert-Amyl methyl ether was used as case study.

Likewise, the evaluation of several reactive HIDiC configurations with an algorithm supported by Genetic algorithms as optimizer was recently achieved (Eyvazi-Abhari, Khalili-Garakani, & Kasiri, 2023). The production of Dimethyl carbonate was used as case study. In this case, the best HIDiC design obtained led to TAC and energy savings of 44% and 42%, respectively.

However, the implementation of these configurations has also been achieved for cryogenic air separation (Wang et al., 2020). The non-uniform heat exchange reduced up 44% the heat exchanger costs in relation with the uniform heat transfer exchange. Similarly, Suphanit (2011) found that the best performance of the HIDiC is obtained with a non-uniform heat distribution along the columns. In fact, the best HIDiC column was determined when the most heat integration (68%–70%) is achieved in the bottom half of the columns. In addition, in comparison with the uniform heat distribution, capital cost reductions of about 32.5% were determined for the non-uniform heat distribution. In this case, the mixture made of propylene/propane is used as case study.

In addition, HIDiC columns have also been implemented to separate azeotropic mixtures, such as the acetone-chloroform-water mixture (Seo, Lee, Lee, & Lee, 2022). The results showed respective reductions of utilities and TAC of 21.79% and 11.32%, in relation with the traditional configuration made of a decanter followed by a PSD distillation.

On the other hand, the high performance of these configurations is supported by good dynamic behavior, at least for the schemes reported. For instance, the examination of an ideal HIDiC configuration under five control strategies was carried out (Nakaiwa et al., 1998). Results disclosed that the five control approaches implemented were able to drive the disturbances and keep the product's specs on their values established. However, the nonlinear process model based control (NPMC) system depicted its superiority over the other control strategies. Later, a novel HIDiC column with heat integration between its overhead product and feed stream was analyzed (Nakaiwa et al., 2000). This configuration conducted to larger control difficulties but the control was achieved by using adequate compression ratios and feed thermal condition. At the same time, the study of a bench-scale experimental HIDiC configuration showed that no special dynamic concerns were experienced during the operation of this configuration (Naito et al., 2000). In fact, authors mention that a smooth operation was achieved. Nevertheless, it has been evidenced a considerable deterioration of the dynamics of the ideal HIDiC due to the influence of pressure distribution (Huang, Matsuda, Takamatsu, & Nakaiwa, 2006). Another study disclosed an increasing of the thermodynamic efficiency but also control difficulties for the totally heat-integrated HIDiC (Huang, Shan, Zhu, & Qian, 2008). Later, researchers showed that an internally heat integrated pressure-swing distillation process (IHIPSD) was able to produce high purity ethanol with good dynamics by implementing PI controllers (Mulia-Soto & Flores-Tlacuahuac, 2011). Even, the controllability of the HIDiC columns has been examined by using the Morari resiliency index, condition number and relative gain array. In this case, authors found that the HIDiC with the best control properties saves concordance with the HIDiC with the minimum TAC (Reza Salehi, Amidpour, Hassanzadeh, & Reza Omidkhah, 2012).

Furthermore, the implementation of a nonlinear wave model analysis on the HIDiC columns showed the dynamics of the transition between two steady states but also the different control properties of the rectifying section and stripping section. In addition, authors showed the influence of the magnitude and direction of the disturbances on the response (Cong, Chang, & Liu, 2015). Likewise, the control properties of the HIDiC have been compared for three control approaches, such as EGMC, PI and R-EGMC. Results corroborated the feasible control of the HIDiC, although the best performance was obtained with R-EGMC approach (Cong, Liu, Deng, & Chen, 2019).

More recently, a channel-type heat exchanger was applied in a heat-integrated distillation column. Simulations showed that this channel-type heat exchanger undergoes a stable dynamic behavior under industrial constraints by implementing PID controllers (Markowski, Trafczynski, & Kisielewski, 2022).

Also, a recent study showed the dynamic behavior of the HIDiC columns using a set of mixtures with low relative volatility and equimolar feed composition. The study was achieved considering the open and closed loop analysis. The results disclosed that the HIDiC columns are controllable technologies and even dynamically better than the conventional sequences (Gutiérrez-Guerra, Segovia-Hernández, & Hernández, 2023).

Although the analysis of the HIDiC columns has been tackled under different perspectives, the impact of the control properties on the energetic and economic performance of the HIDiC columns, under variable feed composition, is a gap in the research. Hence, the novelty of this work lies on determining how the feed composition influences the impact of the dynamic behavior on the energy savings and total cost of optimum HIDiC configurations. Thus, the results presented in this study lead to establish the best integral performance (dynamic, energetic and economic) of these intensified configurations under variable feed composition.

The study was carried out by means of closed-loop analysis of the HIDiC columns using PI controllers and the IAE criterion in Aspen

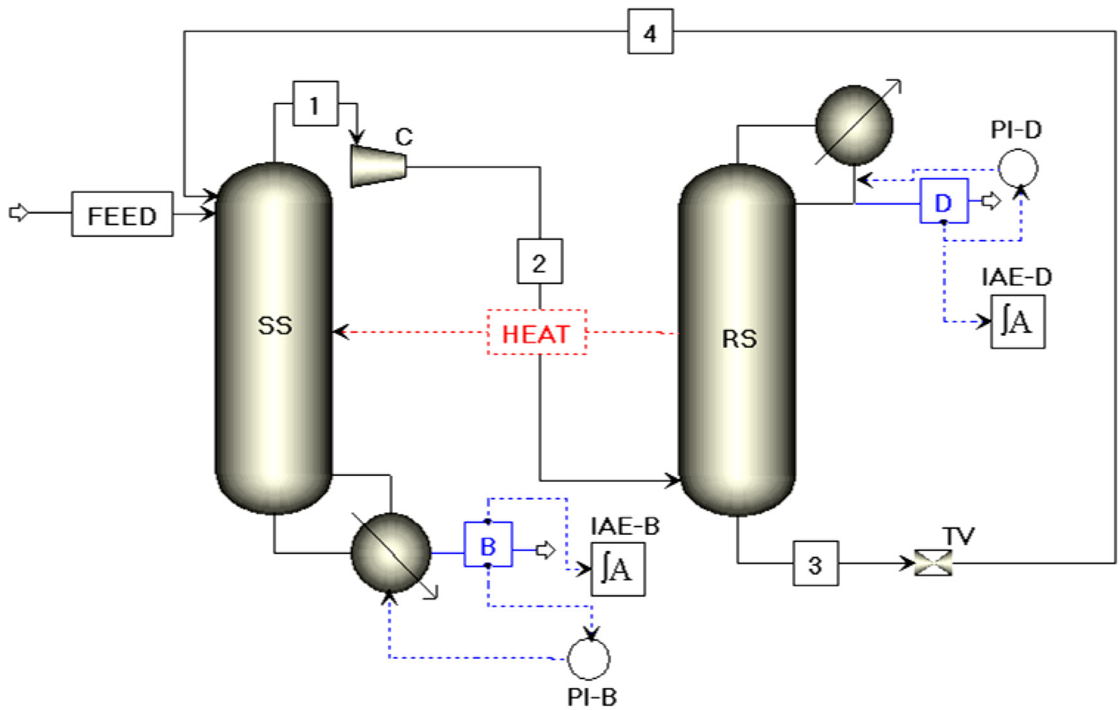


Fig. 2. Flowsheet of HIDiC columns with PI controllers installed.

Table 1
Case studies.

Mixture	Component	α
M1	Cyclohexane/n-Heptane	1.68
M2	Isobutanol/n-Butanol	1.44
M3	n-Octane/Ethylbenzene	1.38
M4	Ethylbenzene/o-Xylene	1.23
M5	m-Xylene/o-Xylene	1.12

dynamics. The HIDiC designs analyzed were optimized using a Boltzmann-based algorithm. The separation of five close-boiling mixtures and three feed compositions were evaluated in this study.

2. Case studies and problem statement

The relationship between the control properties and the energetic and economic performance of the HIDiC configurations was determined for the mixtures described in Table 1.

The hydrocarbon and alcohols mixtures analyzed were selected because they are used as feedstock in the chemical industry and as fuels in the transportation. So, their importance has conducted them to be used as case studies in multiple researches (Barry, Thompson, Baltrusaitis, & Luyben, 2023; Da Silva Filho, Alves, Reus, Machado, & Marangoni, 2018; Deniz Altinkurt, Emre Ozturk, & Turkcan, 2022; Díaz et al., 2016; Nguyen, Hespel, Hoang, & Mounaïm-Rousselle, 2019; Pereira, Dias, Mariano, Maciel Filho, & Bonomi, 2015; Villegas-Uribe, Alcántara-Avila, Medina-Herrera, Gómez-González, & Tututi-Avila, 2021). Particularly, alcohols are mixed with hydrocarbon-based fuels to reduce the environmental pollution. Furthermore, the importance of the mixtures used is highlighted due to that they are close-boiling mixtures characterized by their high energy demands to be purified using traditional distillation configurations. In fact, the largest energetic and economic potential of the HIDiC columns is obtained in the separation of these kinds of systems with low relative volatility (Gutiérrez-Guerra et al., 2016). Therefore, the dynamic analysis of the HIDiC configurations with variable feed composition must be performed to support their economic and energetic potential.

Three feed compositions were evaluated (light component/heavy component): 25mol%/75mol%, 50mol%/50mol% and 75mol%/25mol%, which are denoted (in mole fraction) as: 0.25/0.75, 0.5/0.5 and 0.75/0.25. A feed flow rate of saturated liquid of 100 kmol/h was used.

The HIDiC configurations examined in this work were optimized in energetic and economic terms in previous studies using a Boltzmann-based optimization algorithm (Gutiérrez-Guerra et al., 2016, 2017). The minimization of the TAC was the objective function, while CR, the total number of stages (TNS) and the reflux ratio (RR) were established as optimization variables. The purity and recovery and temperature driving forces ($\Delta T_{RSi-SSi} \geq 1.67$ K) were defined as the constraints of the problem. The same optimization approach was also implemented for the non-equimolar mixtures of Cyclohexane/n-Heptane. Table 2 shows the design and operation variables for the HIDiC and conventional configurations.

The closed-loop process analysis was performed under servo and load disturbance implementing proportional integral controllers (PI) in the HIDiC columns with rigorous hydraulic in Aspen Dynamics. The typical elliptical head geometry was selected for the vessel of the reboiler and condenser while a vertical vessel was chosen for the reflux drum of the HIDiC column. The diameter of these containers was of 2 ft (0.6096 m) whereas the height of the condenser and reboiler vessels and the length of the reflux drum was of 3 ft (0.9144 m). In addition, the centrifugal compressor (C) shown in Fig. 2 has an efficiency of 70% and it is used to keep RS at higher pressure than SS. As it was indicated before, SS is kept at 1 atm. Furthermore, a value of 0.5 was established as the total liquid volume fraction. The simulations were configured as Flow Driven Dyn simulations in Aspen Dynamics in order to manipulate the flows of the HIDiC column using PI controllers. The flowsheet of the HIDiC column with the PI controllers installed is depicted in Fig. 2.

Table 2
Design and operation variables of the HIDiC and conventional configurations.

Mixture	Design	Conventional columns			HIDiC configurations		
		Feed composition			Feed composition		
		0.25/0.75	0.5/0.5	0.75/0.25	0.25/0.75	0.5/0.5	0.75/0.25
M1	TNS	40	56	36	40	56	36
	CR	–	–	–	1.80	1.86	1.68
	RR	6.72	3.06	2.93	1.90	0.38	0.68
	Purity	0.9951	0.9951	0.9947	0.9950	0.9949	0.9947
	Recovery	0.9951	0.9951	0.9947	0.9950	0.9949	0.9947
	Heat duty (kJ/h)	5.80E+06	6.13E+06	8.82E+06	2.24E+06	2.27E+06	3.94E+06
	TAC (USD/year)	5.52E+05	6.10E+05	7.70E+05	9.2E+05	8.04E+05	8.85E+05
M2	TNS	56	72	80	56	72	80
	CR	–	–	–	1.87	1.76	2.18
	RR	11.65	5.27	3.70	0.98	0.084	0.19
	Purity	0.9948	0.9951	0.9948	0.9948	0.9950	0.9950
	Recovery	0.9948	0.9952	0.9948	0.9948	0.9952	0.9950
	Heat duty (kJ/h)	1.23E+07	1.23E+07	1.39E+07	1.84E+06	2.20E+06	3.60E+06
	TAC (USD/year)	1.13E+06	1.18E+06	1.32E+06	1.24E+06	1.16E+06	1.25E+06
M3	TNS	90	74	90	90	74	90
	CR	–	–	–	2.29	1.34	1.59
	RR	24.00	23.56	12.40	3.33	9.63	0.68
	Purity	0.9949	0.9949	0.9948	0.9948	0.9952	0.9948
	Recovery	0.9949	0.9949	0.9948	0.9948	0.9951	0.9948
	Heat duty (kJ/h)	2.05E+07	4.05E+07	3.33E+07	3.55E+06	1.86E+07	4.35E+06
	TAC (USD/year)	1.96E+06	3.33E+06	3.01E+06	1.73E+06	2.73E+06	2.21E+06
M4	TNS	94	78	90	94	78	90
	CR	–	–	–	1.51	1.46	1.47
	RR	22.30	13.20	7.00	2.10	2.55	0.12
	Purity	0.9949	0.9950	0.9948	0.9949	0.9953	0.9950
	Recovery	0.9949	0.9953	0.9948	0.9949	0.9947	0.9950
	Heat duty (kJ/h)	1.92E+07	2.54E+07	2.00E+07	2.64E+06	6.38E+06	3.01E+06
	TAC (USD/year)	2.00E+06	2.41E+06	2.08E+06	2.11E+06	2.42E+06	2.12E+06
M5	TNS	130	138	134	130	138	134
	CR	–	–	–	1.5	1.56	1.51
	RR	74.98	33.92	26.40	9.9	4.25	2.37
	Purity	0.9952	0.9953	0.9952	0.9947	0.9950	0.9948
	Recovery	0.9952	0.9953	0.9952	0.9947	0.9950	0.9948
	Heat duty (kJ/h)	6.34E+07	7.22E+07	6.95E+07	9.30E+06	9.59E+06	8.78E+06
	TAC (USD/year)	5.97E+06	5.32E+06	6.50E+06	5.10E+06	5.68E+06	5.52E+06

To determine the dynamic behavior of the HIDiC configurations, the corresponding closed-loop control arrays using PI controllers were firstly assembled (see Fig. 2). One PI controller was placed in the bottoms stream of the HIDiC column and the other one was added to the Distillate stream. Secondly, the closed-loop control arrays were configured by introducing the setpoint to be tracked by the PI controller. In this case, the value of the setpoint for each PI controller is determined by multiplying the current composition (rich component for the respective stream) by 0.99. This value represents 1% of disturbance of the rich component (either distillate or bottoms) regard the original purity value. This percentage of disturbance was established in order to reduce the non-linearity of the process (Skogestad & Morari, 1998). Thirdly, the tuning of the PI controllers takes place. In this point, multiple gain (Kc) and integral time (τ) pairs are evaluated in the PI controllers. So, for each gain and integral time pair, the simulation is run and the setting of the composition to the setpoint is performed. Here, the composition setting to the setpoint is carried out by manipulating the reflux ratio when the disturbance is applied in the rich product of the distillate. Similarly, the composition setting of the rich product of the bottoms is achieved by manipulating the reboiler duty. So, the size of the control actions performed by the PI controller will depend on the deviation between the current composition and the setpoint.

Furthermore, the IAE index was used to determine the control properties of the HIDiC configurations. This index is represented as $\int$A in the flowsheet shown in Fig. 2.

As shown in Eq. (1), the IAE is defined as the Integral Absolute Error, where $\varepsilon = \text{ysp(t)} - \text{y(t)}$, which represents the error (deviation) between the setpoint (ysp(t)) and the response y(t) of the process variable (Stephanopoulos, 1984). In this case, the products composition is the process variable.

$$IAE = \int_0^\infty |\varepsilon(t)|\, dt \tag{1}$$

IAE criterion was chosen because small errors of the composition regard the setpoint are expected due to the small disturbance induced. So, the best control properties will be given by the lowest values of the IAE index obtained through the tuning of the PI controller.

On the other hand, the control approach presented in this paper was established considering that the products quality (design specs) is the main goal tracked in the operation of a distillation process. In addition, the multivariable operation of these separation technologies might conduct to diverse composition disturbances of the products, derived from unexpected or programmed operational settings. Therefore, in this work is tracked the capability of the HIDiC columns to deal with composition disturbances using PI composition controllers.

In this case, PI controllers were implemented because they are the most used controllers in the chemical industry due to their cost-benefit, that is, their good performance and relatively economic assembling (Baghmisheh, Shahrokhi, & Bozorgmehri, 2010; Luyben & Yu, 2008).

On the other side, notice that this study is limited to determine the dynamic behavior of HIDiC configurations using two PI controllers only. Therefore, a complementary dynamic analysis to evaluate the influence of other disturbances (e.g. feed flowrate and feed composition) on the products composition should be carried out.

Similarly, the dynamic performance of the HIDiC columns under other control approaches, such as cascade control using PI controllers and model predictive control (MPC), could be examined (Qian et al., 2019). Furthermore, notice that there exist some practical difficulties to perform the direct composition control due to high cost of online composition analyzers and delays in the composition data flow in real time (Qian et al., 2019). In fact, in practice, the composition control is indirectly made through temperature control (Kong, Zhang, Cui, & Sun, 2020; Qian et al., 2019; Wu & Chien, 2022). Notice, however, that the control approach used in this work was supported because the simulation study using Aspen Plus Dynamics is not constrained by the practical concerns (technological, operational and costs) described before. So, although this study does not provide a completely disclosed dynamic performance through the PI controllers presented, the results obtained will give a preliminary dynamic estimation to achieve more rigorous dynamic analysis of these configurations. In other words, the results obtained will provide valuable guidelines to be considered in further studies under other control structures implemented in the HIDiC configurations.

The integral analysis of the performance of these configurations was conducted considering the control properties and the energetic and economic behavior simultaneously. Here, TR represents the economic and energetic performance of the HIDiC configurations. This factor is determined by the summation of Qr plus TACr for each feed composition of each mixture. TACr is defined as the ratio between the TAC of the HIDiC column and the TAC of its equivalent conventional sequence (non-optimized) with the same TNS (TACr = TAC HIDiC/TACconv). Similarly, Qr represents the ratio between the Heat duty of the HIDiC column and Heat duty of the conventional column (non-optimized) with the same TNS (Qr = Heat duty HIDiC/Heat duty conv). The data used to compute Qr and TACr were taken from Table 2.

3. Results and discussion

Results presented in Fig. 3 show that similar control properties were determined for the mixtures with lower α (M3-M5), see Fig. 3c–e. Nevertheless, this trend is considerably different to the behavior depicted by the mixtures M1 and M2, Fig. 3a–b. In fact, the lowest IAE values for these mixtures (M1 and M2) lie on opposite ends, i.e., the lowest IAE value for the mixture M1 was obtained for a feed composition of 0.25/0.75 while the lowest IAE value for the mixture M2 was obtained for a feed composition of 0.75/0.25. However, the lowest IAE values for the mixtures M3-M5 (Fig. 3c–e) were determined for feed compositions between 0.25/0.75 and 0.5/0.5. Hence, a more uniform tendency was experienced by the HIDiC columns used to separate the mixtures with lower α. Besides, it is observed that the highest IAE values were two orders of magnitude larger for some feed compositions of the mixture with the lowest α (mixture of xylenes) in relation with the other mixtures. This fact denotes that greater control work is required for the HIDiC columns of M5.

On the other hand, the analysis of Table 3 shows that the HIDiC columns with the best control properties (BCP) do not agree with the HIDiC columns with the best energetic and economic performance for the mixtures analyzed. In fact, the best control properties were identified for equimolar feed composition for the mixtures M3 and M4 and a feed composition of 0.25/0.75 for the mixture M5. However, the best energetic and economic performance for these mixtures was determined for a feed composition of 0.75/0.25. Furthermore, it is interesting to note that the best energetic and economic performance of the HIDiC columns saves concordance with the worst control properties (WCP) for these mixtures.

In addition, it is observed that the best control properties for the mixture M1 were obtained for a feed composition of 0.25/0.75 but the best energetic and economic performance was determined for a feed composition of 0.75/0.25. Notice also that the worst control properties for this mixture were found for the equimolar feed composition.

Besides, it is shown that the best dynamic behavior for the mixture M2 was determined for a feed composition of 0.75/0.25 but the best energetic and economic performance was obtained in a feed composition of 0.5/0.5. Nevertheless, the worst dynamic behavior was determined for a feed composition of 0.25/0.75.

Thus, the HIDiC configuration with the best control properties for M1 (0.25/0.75) is the HIDiC design with the highest TACr cost but provides similar energy saving as the HIDiC design with the largest energy saving (Qr). In fact, TR for this configuration is 2.06. The second best control (SBCP) is the HIDiC column with a feed composition of 0.75/0.25, which shows the lowest TACr but the largest Qr. At the same time, it is observed that the configuration with the worst control properties is the HIDiC column with an equimolar composition. Nevertheless, the largest energy saving has been determined for this HIDiC configuration and its TAC is slightly larger than the minimum TAC found for this mixture.

Hence, considering the cost-benefit (TR = 1.6) and dynamic behavior, the HIDiC with a feed composition of 0.75/0.25 is the most adequate option to carry out this separation.

Furthermore, the integral analysis achieved for M2 indicates that the HIDiC column with the best control properties provides the largest Qr but the lowest TACr regarding the other compositions. Observe also that the second best control properties were determined for the HIDiC with an equimolar composition, whose TACr and Qr lie between the values of the other feed compositions. In addition, the worst control properties were found for the HIDiC with a feed composition of 0.25/0.75. This configuration provides the largest TACr but similar Qr as the equimolar composition. Thus, the best option to perform the separation is the HIDiC with a feed composition of 0.5/0.5, with a TR value of 1.16.

Additionally, the analysis for M3 indicates that the HIDiC configuration with the worst control properties (0.75/0.25) is that with the lowest TACr and Qr, but the best dynamic properties were determined for the configuration with equimolar feed composition. As we can see, this column has the largest Qr but an average TACr in relation with the other feed compositions. In this case the SBCP were determined for a feed composition of 0.25/0.75. However, this configuration has similar Qr as the HIDiC with a feed composition of 0.75/0.25 but a relatively larger TACr. So, the most convenient separation for this mixture is achieved using a feed composition of 0.25/0.75, which has a TR of 1.05.

As it was described before, the HIDiC sequence with the best control properties for (M4) was determined with equimolar feed composition. This configuration has the largest Qr but the lowest TACr in comparison with the other feed compositions. On the other hand, it is observed that the SBCP is given by the HIDiC column with a feed composition of 0.25/0.75, which presents the lowest Qr but larger TACr than the other configurations. Besides, the worst control properties are again found for the HIDiC with a feed composition of 0.75/0.25. This sequence operates with a similar Qr as the HIDiC with a feed composition of 0.25/0.75, but lower TAC. Consequently, taking into account the energy consumption and TAC (TR = 1.2) and control properties, the best configuration to perform the separation is the HIDiC with a feed composition of 0.25/0.75.

In addition, in concordance with the mixtures M3 and M4, the analysis for the mixture M5 showed the worst dynamic performance for the HIDiC with a feed composition of 0.75/0.25. Nevertheless, as it can be observed, this configuration presents

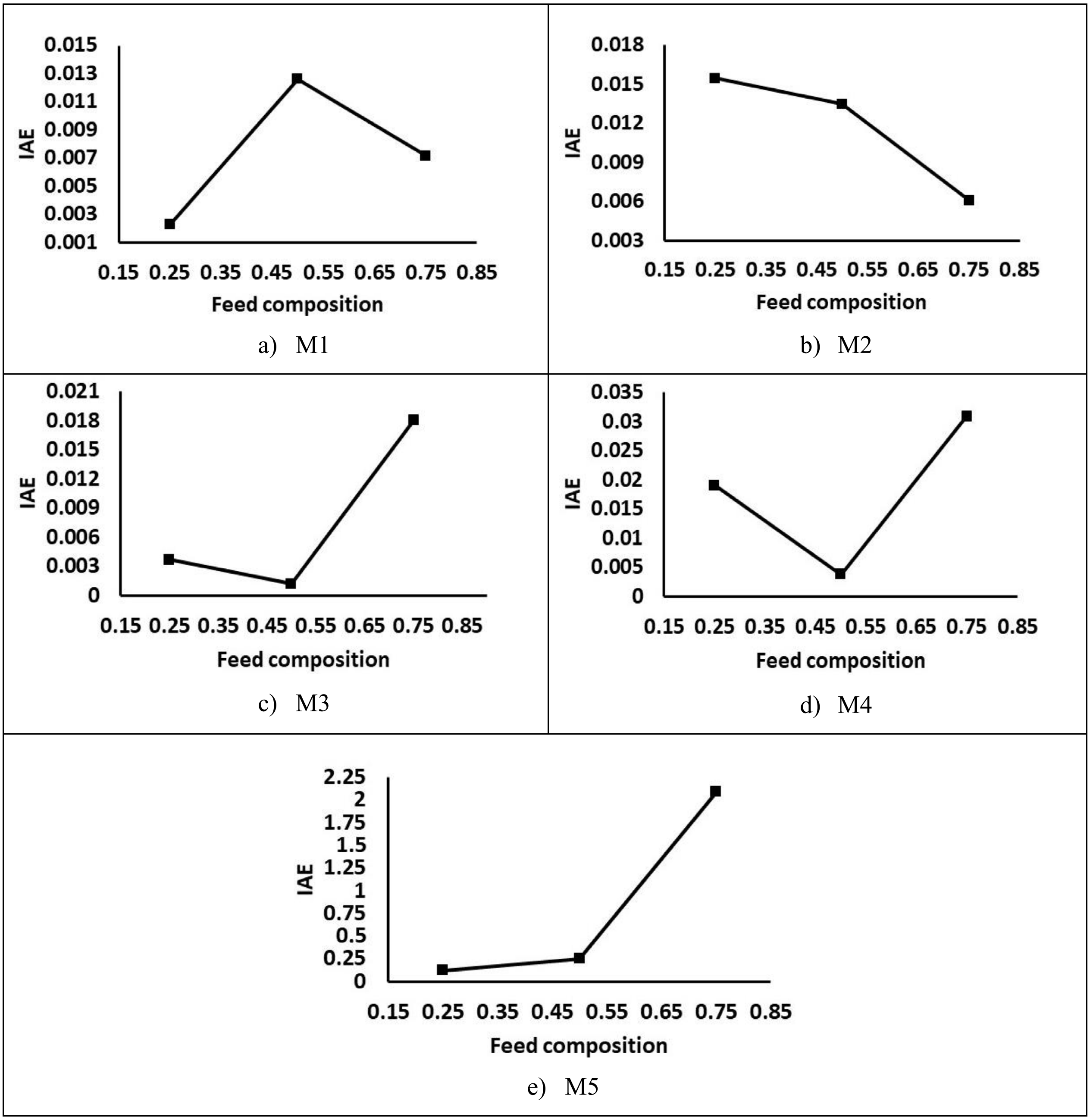


Fig. 3. IAE (IAE distillate plus IAE bottoms) for each feed composition.

Table 3
Dynamic behavior versus energetic and economic performance of the HIDiC columns.

Mixture	Feed composition						Feed composition			Dynamic performance		
	0.25/0.75		0.5/0.5		0.75/0.25		0.25/0.75	0.5/0.5	0.75/0.25			
	Qr	TACr	Qr	TACr	Qr	TACr	TR			BCP	SBCP	WCP
M1	0.39	1.67	0.37	1.32	0.45	1.15	2.06	1.69	1.6	0.25/0.75	0.75/0.25	0.5/0.5
M2	0.15	1.10	0.18	0.98	0.26	0.95	1.25	1.16	1.21	0.75/0.25	0.5/0.5	0.25/0.75
M3	0.17	0.88	0.45	0.82	0.13	0.73	1.05	1.27	0.86	0.5/0.5	0.25/0.75	0.75/0.25
M4	0.14	1.06	0.25	1.00	0.15	1.02	1.2	1.25	1.17	0.5/0.5	0.25/0.75	0.75/0.25
M5	0.15	0.86	0.13	1.07	0.13	0.85	1.01	1.2	0.98	0.25/0.75	0.5/0.5	0.75/0.25

the lowest Qr and also the lowest TACr. Likewise, the SBCP were determined for the HIDiC with a feed composition of 0.5/0.5. As before, this configuration shows the lowest Qr as the HIDiC with a feed composition of 0.75/0.25 but a TACr considerably larger. Furthermore, the best control was determined for the HIDiC configuration with a feed composition of 0.25/0.75. This configuration has a TACr and Qr similar to the HIDiC with feed composition of 0.75/0.25. Hence, it is obvious that the best HIDiC configuration to achieve this separation is the HIDiC configuration with a feed composition of 0.25/0.75 with TR of 1.01.

Thus, these results show that the best compromise between control properties, energy consumption and TAC of the HIDiC configurations is given for a feed composition of 0.75/0.25 for the mixture M1 and a feed composition of 0.5/0.5 for the mixture M2. Moreover, the HIDiC columns that provide the best compromise for the mixtures M3-M5 were those with a feed composition of 0.25/0.75.

On the other hand, the behavior shown in Fig. 4 indicates that the HIDiC columns were able to deal with the disturbances and reach steady-state using PI controllers.

Besides, the results show that most HIDiC columns experienced a relatively high level of sensitivity (large gains) and required a relatively short integral time to attenuate the oscillations experienced by the products composition. Particularly, it is observed that more balanced control efforts (between the integral action and the proportional action) were required in a couple of HIDiC columns (bottoms of M3 and distillate of M5). In these cases, both short integral time and small gains (in comparison to the other control loops) were used for the corresponding PI controllers. Nonetheless, large settling time was observed due to the sensitivity level experienced. On the other side, it is notorious that the rich product of bottoms for M1 and M5 experienced low sensitivity and a long integral time was required to get the steady-state. In addition, it is interesting to note that the relatively large control effort experienced by M5 agrees with the largest IAE value determined for this mixture. So, special attention must be directed to the dynamics of the mixtures with α near enough to unity. So, these results demonstrate that the composition control of the HIDiC columns under study was well tackled by the control approach proposed.

Notice however, that despite these valuable findings, the dynamic behavior of the HIDiC columns will be completely described when the examination of other disturbances (e.g. feed flowrate and feed composition) on the products composition and the implementation of other control approaches take place.

These trends reflect the level of sensitivity of the columns as a consequence of the amount of internally integrated heat constrained by temperature driving forces between RS and SS. In fact, Table 4 shows that as α reduces, the level of energy integration (Qint.) tends to decrease with the reduction of the feed composition of the mixtures. For instance, the best integral performance for the HIDiC of the mixture M1 (feed composition of 0.75/0.25) is powered by a relatively large internal heat integration in comparison with the other feed compositions. Nonetheless, the best integral behavior of the HIDiC column for the mixture M2 (equimolar feed composition) was obtained with a mean level of internal heat integration, in relation with the other feed compositions. Besides, notice that the best integral performance for the HIDiC configurations of the mixtures with lower α (M3-M5) and feed compositions of 0.25/0.75, are powered by the minimum levels of internal heat integrated (M3 and M5) or tend to the minimum internally heat integrated value (such as the mixture M4) in relation with the other feed compositions.

Thus, this analysis evidences that the best integral performance is obtained by increasing the internally heat-integrated for large feed compositions for the light component as α rises. Likewise, the HIDiC columns with the best integral performance used to separate the mixtures with $\alpha < 1.4$ are supported by low feed compositions for the light component and reductions in the internally heat integrated in relation with the other feed compositions.

On the other side, the correlation between the level of internally heat integrated and the feed composition of the mixtures is supported by the behavior depicted in Figs. 5–6. Here, it is observed that the trend of the IAE of the HIDiC columns with the best integral performance (Fig. 5) follows a similar trend to the level of internally heat integrated (Fig. 6) for the corresponding feed composition of each mixture. Therefore, this fact validates the direct correlation between the dynamic behavior and the internally heat integrated from RS to SS for the corresponding feed composition of the mixtures under study.

Table 4
Qint. for the HIDiC columns.

Mixture	Feed composition		
	0.25/0.75	0.5/0.5	0.75/0.25
	Qint. (kJ/h)		
M1	9 486 212.87	7 074 605.10	11 309 583.30
M2	20 366 680.80	15 026 765.10	10 557 802.10
M3	13 952 818.64	22 464 730.00	32 457 698.10
M4	34 326 008.20	38 770 314.00	33 231 708.90
M5	112 581 867.00	129 315 322.00	130 856 756.00

Hence, this behavior shows that the regulation of the internally heat integrated is a fundamental issue that must be taken into account to keep an adequate integral performance of the HIDiC configurations. Consequently, it is required to carry out an adequate control of the temperature driving forces generated between RS and SS. So, these results conduct to establish that the internal flows (vapor and liquid) have higher impact on the control properties than the external flows for systems with variable feed composition. At the same time, these vapor and liquid flows undergo a direct relationship with the amounts of integrated heat, see Table 5.

Results of Table 5 reveal that a relatively low energy fraction used by the HIDiC configurations is given by the reboiler and also removed by the condenser. As it is observed, the contribution of the reboiler (addition of heat) and the condenser (heat removal) is less than 20% for most cases. Therefore, it is then demonstrated that the dynamic, energetic and economic performance of the HIDiC configurations is strongly influenced by the internal heat integration and the feed composition. On the other hand, these results indicate that the harnessing of the largest energetic and economic benefits will be particularly constrained by the dynamics of the HIDiC columns with α close to unity for the feed compositions analyzed.

So, the results presented provide an important reference for guiding the dynamic study of HIDiC columns for separating other close-boiling mixtures. In fact, an analogous dynamic behavior is expected for HIDiC columns used to separate mixtures with similar relative volatility to the range presented in this work. However, next issues must be considered if the dynamic analysis of HIDiC columns for separating mixtures with a considerably different value of α is carried out: (a) By one side, larger compression ratios are used for systems with larger relative volatilities (e.g. $\alpha > 2.4$). Nevertheless, the heat integration is less harnessed and the cost-benefit of the HIDiC columns tends to be reduced and even lost. In fact, if CR is minimized for these mixtures, a minimum amount of energy will be integrated. In this case, the control properties of the HIDiC columns might tend to the dynamic behavior of the conventional columns. (b) On the other side, if α reduces further than 1.13 but larger than 1, a low value of CR is estimated but the cost-benefit could be underestimated due to that considerably larger control problems for the HIDiC columns are expected. This performance is a consequence of the close azeotropic behavior of the mixtures with α close enough to unity.

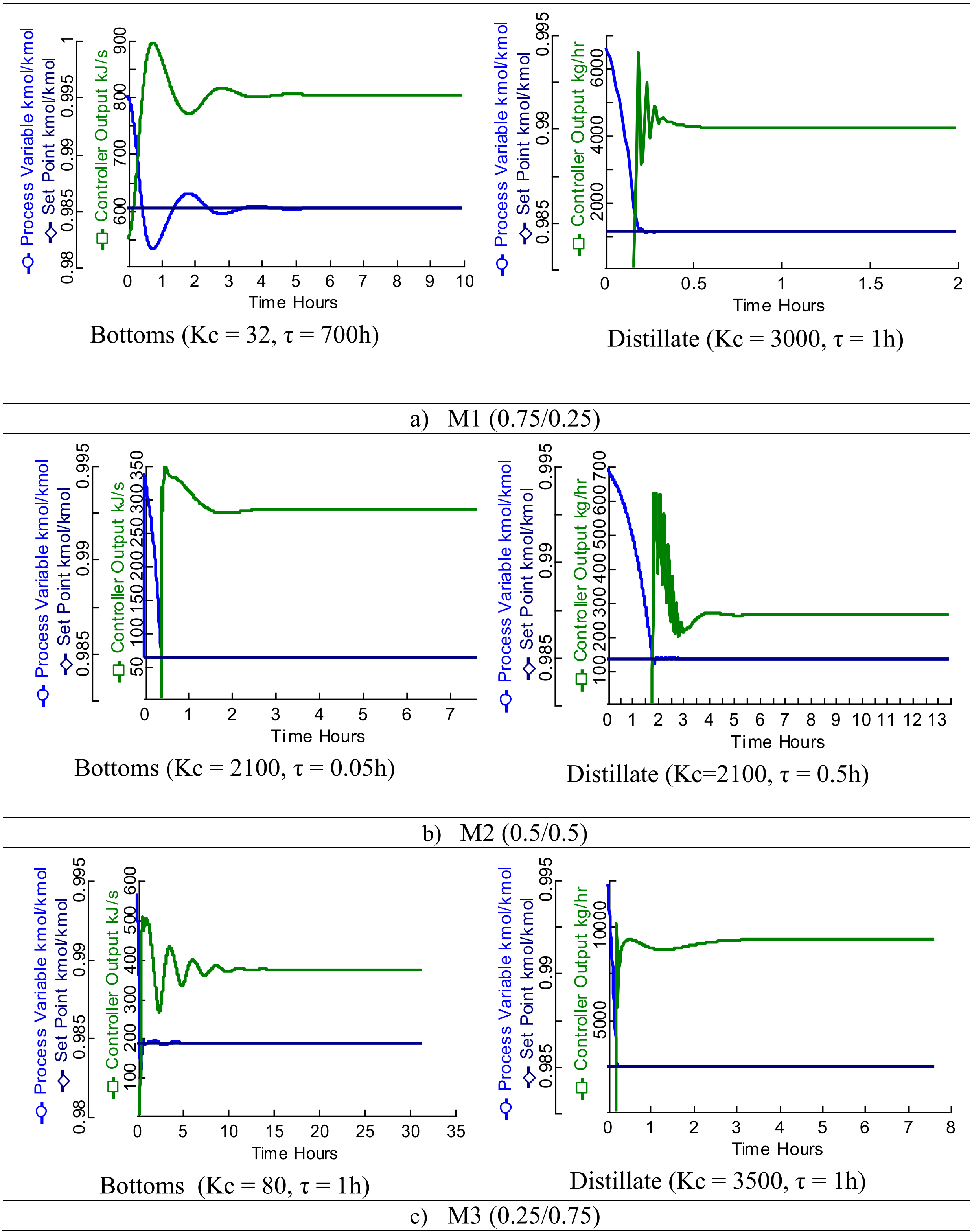
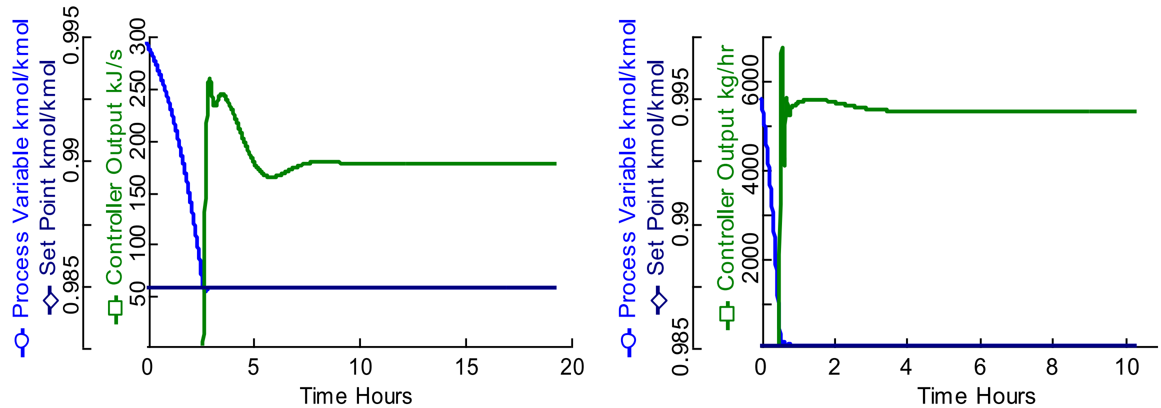


Fig. 4. Closed-loop dynamic response.

4. Conclusions

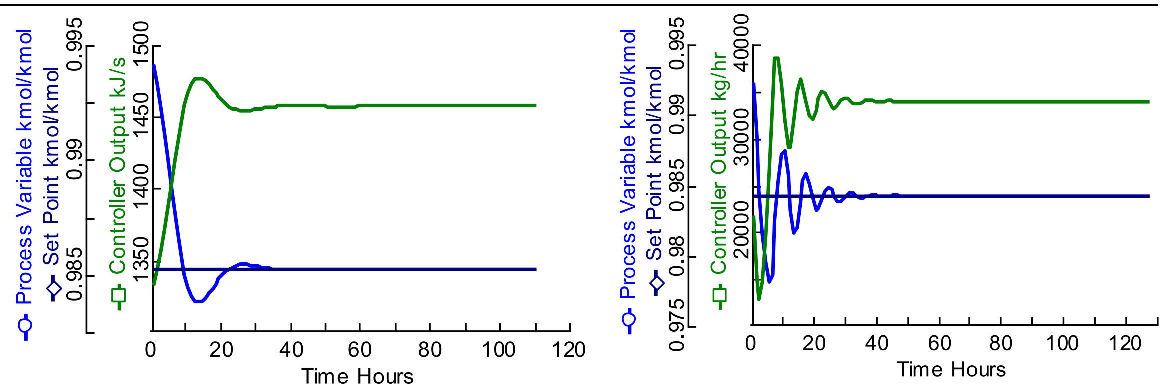
In this paper, the impact of the control properties on the energetic and economic performance of Heat-Integrated Distillation Columns under variable feed composition is presented.

The separation of five close-boiling binary mixtures was carried out. The HIDiC columns used as case studies are the optimal HIDiC sequences rigorously optimized in previous studies (Gutiérrez-Guerra et al., 2016, 2017). The evaluation of three feed compositions (0.25/0.75, 0.5/0.5, 0.75/0.25) for each mixture



Bottoms (Kc = 700, τ = 1h) Distillate (Kc = 2000, τ = 3h)

d) M4 (0.25/0.75)



Bottoms (Kc = 10, τ = 3500h) Distillate (Kc = 3, τ = 3h)

e) M5 (0.25/0.75)

Fig. 4. (*continued*).

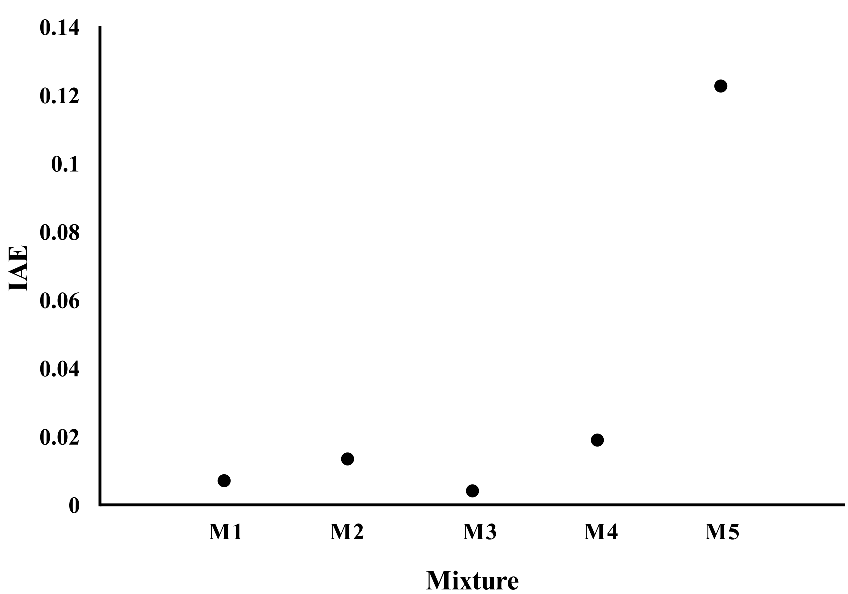


Fig. 5. Trend of IAE for the HIDiC columns with the best integral performance.

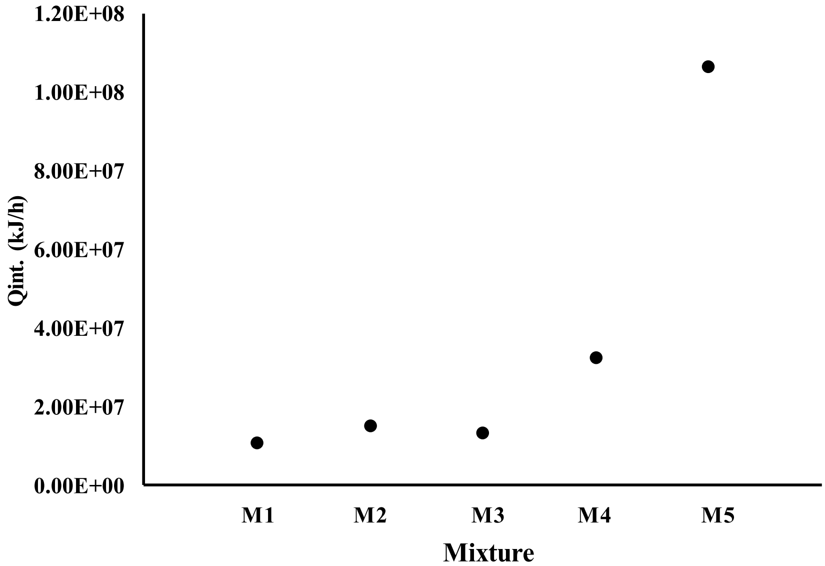


Fig. 6. Trend of Qint. for the HIDiC columns with the best integral performance.

Table 5
Heat distribution in the HIDiC columns with the best integral performance.

Mixture	Feed composition	Qint. (kJ/h)	QReb. (kJ/h)	QCond. (kJ/h)	Qratio-SS	Qratio-RS
M1	0.75/0.25	11 309 583.30	2 912 632.04	3 624 045.11	0.205	0.243
M2	0.5/0.5	15 026 765.10	1 043 286.64	2 165 327.10	0.065	0.126
M3	0.25/0.75	13 952 818.64	1 375 869.35	3 443 004.41	0.090	0.198
M4	0.25/0.75	34 326 008.20	657 696.68	2 615 438.98	0.019	0.071
M5	0.25/0.75	112 581 867.00	2 914 553.16	9 597 973.56	0.025	0.079

was performed. The control properties were obtained using the closed-loop process and the IAE criterion.

Based on the results obtained, next conclusions are highlighted:

The feed composition is an important operation variable that must be considered to obtain the best performance of the HIDiC configurations. However, the performance must be determined through an integral analysis, considering simultaneously the energetic and economic behavior but also the dynamics of these configurations.

Furthermore, it is also concluded that the value of the IAE index saves concordance with the level of integrated energy. Consequently, the level of intensification (energy integration) must be balanced in order to obtain a favorable cost-benefit and better dynamic properties for these configurations.

Likewise, special attention must be directed to the separation of mixtures with α close enough to unity because a particularly large control effort was found for these kinds of configurations.

Thus, the dynamics determined for the HIDiC columns could be used as a reference to disclose a more generalized dynamic performance by implementing other control structures. At the same time, the dynamic behavior shown might be taken into account to determine the integral performance of HIDiC columns used to separate other close-boiling mixtures.

CRediT authorship contribution statement

R. Gutiérrez-Guerra: Writing – original draft, Visualization, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **J.G. Segovia-Hernández:** Writing – review & editing, Software.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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