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Heat integration and process improvement of a batch distillation unit using a gradual feeding strategy: A case study on MIBK-water separation

Saber Niazi *, José Antonio Díaz-López, Antonio Nieto-Márquez *

Departamento de Ingeniería Mecánica, Química y Diseño Industrial. Escuela Técnica Superior de Ingeniería y Diseño Industrial, Universidad Politécnica de Madrid, Ronda de Valencia 3 28012 Madrid, Spain

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ABSTRACT

This work focuses on upgrading a batch distillation unit in terms of energy efficiency and production capacity. Dehydration of methyl isobutyl ketone (MIBK) is performed as a case study. Since the MIBK-water mixture forms a heteroazeotrope, a decanter is applied to facilitate the separation process. The unit performance is evaluated in terms of specific product flow (SPF) and specific energy cost (SEC). Studying the impact of feed quantity in the range of 20 to 80 kg showed that due to the almost equal holdup loss, a larger batch feed quantity results in higher energy efficiency and production performance. Gradual feeding policy with different feeding strategies and locations (i.e., top feeding and bottom feeding) is also assessed in detail and compared with the conventional batch distillation process. Also, three feeding rate profiles (increasing, fixed, and decreasing) with varying feeding durations are evaluated in order to reach the optimal feeding time and profile. Overall, gradual feeding is found to be an efficient approach to upgrade the unit operation in terms of energy efficiency and production rate. Top feeding (also known as batch stripping or inverted batch distillation) has proved to be a more efficient policy for MIBK-water separation over bottom feeding. In addition, the decreasing feed flow rate scenario offers a more efficient operation compared to other feed rate profiles. Accordingly, employing the top feeding policy with a decreasing feed rate profile can lead to a 10 % improvement in production rate and energy cost over a conventional batch distillation unit equipped with a decanter. Moreover, based on the gradual feeding approach, a novel and easy-to-apply strategy for heat integration and recovery in the batch distillation process is proposed, and its potential is assessed for different feeding scenarios. The proposed strategy is also found to be significantly effective in process intensification and acceleration. Applying this strategy to a batch distillation unit with top feeding at a fixed feed rate offers over 47 % improvement in energy efficiency and production rate compared to a conventional batch distillation unit equipped with a decanter.

1. Introduction

Methyl Iso-Butyl Ketone (MIBK) is a versatile solvent with a broad range of industrial applications. Its outstanding dissolution properties, biodegradability, and limited water solubility make it valuable in numerous chemical processes and in the industrial production of pharmaceuticals, paints, rubber, pesticides, cleaning solvents, etc. [1,2]. Specifically, it is used as a solvent in the paint industry, where it ends up mixed with water after use. There are also some other cases in which MIBK is polluted by a small fraction of water and needs to be recovered [3,4]. The low solubility of water in MIBK (about 2 % at room temperature and atmospheric pressure) allows for the mechanical removal of the major fraction of water. The remaining binary mixture forms a heteroazeotrope, similar to the water-tert-butanol (2-methyl-2-propanol) binary mixture [5] that needs to be removed by a suitable unit operation such as heteroazeotropic distillation, in continuous or batch mode. A batch distillation unit (BDU) is a suitable candidate for separation of MIBK-water mixture, especially in small production capacities and low budget for initial investment. The advantages of batch over continuous distillation can be listed as low capital cost, applicability in small scales, product traceability, possibility to cope with different separation tasks, offering a wide range of products using the same unit, availability of various configurations, and ability to handle high solid content [6–8]. Batch distillation is extensively used for purification goals or solvent recovery in the production of pharmaceuticals, polymers, fine and high-value market chemicals, and biochemical products

* Corresponding authors.
E-mail addresses: s.niazi@upm.es (S. Niazi), antonio.nieto@upm.es (A. Nieto-Márquez).

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[9,10].

Production rate and energy efficiency of a BDU, employed for separation of a heteroazeotropic mixture, can be upgraded by integrating a mechanical liquid–liquid separator into the unit. Zhang et al. [11] proposed using heteroazeotropic batch distillation for phenol dehydration as an alternative to direct distillation, providing higher product quality and approximately 20–25 % energy savings. Adding a decanter to the BDU applied for MIBK dehydration has demonstrated successful operation, along with improvements in energy efficiency and production rate. To characterize the employed BDU and optimize the unit performance, effects of start-up policy, reflux ratio, decanting quality, column section height, condenser temperature, and feed quantity have been studied previously. After development and characterization of an efficient unit operation based on batch distillation, a particular gradual feeding policy on unit performance was assessed, showing its positive impacts on the unit performance, including a higher production rate and lower energy consumption [12–14]. In pursuit of our goal to develop an efficient unit operation for MIBK dehydration, developing a feasible and easy-to-apply heat integration approach to improve the energy and separation efficiency of the BDU is aimed in this study.

There are different approaches developed for heat integration and process intensification of a BDU, among which heat pumps have gained more attention recently. As representative examples, Nair and Raykar [15] used a two-stage vapor recompression (VRC) heat pump to enhance the separation of a ternary mixture of hexanol, octanol, and decanol, observing a 52 % energy saving and a 12.2 % total annual cost reduction. Radhika et al. [16] incorporated a double-stage VRC heat pump into a BDU to integrate heat and separate the ternary mixture. Their proposed integrated configurations resulted in a 41.7 % lower energy consumption compared with a conventional BDU. Gandu et al. [17] proposed a heat pump-assisted batch distillation unit for separation of a ternary mixture aiming for reduced cost and carbon emissions. A multi-stage VRC algorithm is introduced as an alternative for the single-stage VRC approach due to its challenges with high vapor compression ratio (>3.5). They found that the feed composition determines each approach's cost-effectiveness, with the highest reported total annual cost reduction in their work being about 10 %. Kazemi et al. [18] proposed using the bottom flashing heat pumps as an alternative to VRC heat pumps. They reported a total annual cost saving of 19 %, using a flashing heat pump and lower annual costs in the range of 4.2–10.9 % compared to the equivalent process with vapor recompression heat pumps. Modla and Lang [19] conducted a study on integrating different heat pump systems in batch distillation units, concerning the economic feasibility of heat integration and payback periods. According to their evaluation, direct application of VRC was not economically feasible, as the minimum payback period was over 10 years, while they managed to reduce it to about seven years by adding a heat exchanger. A conclusion extracted from these studies is that, while heat pumps for heat integration in a BDU offer significant improvements in energy efficiency, they face key challenges, including high capital costs, long payback periods, and complexity in design, control, and operation [19–21].

Alternatively, external energy integration by feed stream heating/flashing stands as a simple and practical approach in continuous distillation [22,23]; however, it is not feasible in batch distillation due to the absence of a feed stream. Building on the proven potential of gradual feeding to enhance unit performance in a previous study [14], this study advances the development by evaluating various feeding strategies, including feeding locations and feed rate profiles, to identify the optimal operating policy in terms of energy cost and production capacity. Also, emerging a feed stream in the batch distillation unit unlocks the potential for heat recovery, as this feed stream can be easily heated by serving as a coolant in the condenser. Evaluating the potential of heat recovery for upgrading the batch distillation unit demonstrates a remarkable breakthrough in the unit's energy efficiency and production capacity.

2. Methodology and study plan

2.1. Simulation procedure

The simulations are conducted using the commercial package Aspen Plus V.14®, applying UNIQUAC model and the BatchSep module. The MIBK-water system exhibits significant deviations from ideality, particularly due to polarity differences between the two components and hydrogen bonding interactions. Given the moderate operating pressure (<10 bar) and the absence of electrolytes, the UNIQUAC model was selected to simulate the MIBK-water system due to its proven capability to handle highly non-ideal and polar liquid mixtures. While the UNIQUAC accuracy strongly depends on high-quality binary parameters (BIP), the validated parameters available in the Aspen Plus database ensure accurate simulation. Fig. 1a shows the phase diagram of the MIBK-water mixture predicted by UNIQUAC together with experimental values provided by NIST Thermo Data Engine (TDE) database [24] indicating the high accuracy of this package in predicting the MIBK-water mixture behavior. Further details on the binary mixture of MIBK-water and the methods applied for simulation are available in our previous studies [13,14]. The goal is to dehydrate a 98 wt% MIBK solution, commonly found as a residue of paint industries, to achieve a minimum purity of 99.8 wt% as standard purity of MIBK for reusing it as solvent.

As Fig. 1b indicates, a conventional batch distillation unit consisting of (1) a still/pot that contains the feed and embeds the reboiler, (2) the column section including mass transfer media (trays or packed beds), and (3) a condenser. Some other accessories, such as a reflux drum, a decanter, a feed tank, and distillate collection tanks, might also be added to the unit, depending on the operation policy. The technical features of the batch distillation unit are presented in Table 1, and the operating conditions defined in the simulation are presented in Table 2. The feed temperature is 25°C, and considering the still capacity, the feed quantity can vary in the range of 20 to 80 kg. The condenser temperature is set to 85°C providing a total condenser condition, and operation is conducted in atmospheric pressure. Reboiler duty (heating rate) is set to ensure processing the pot total feed capacity in less than 8 h, and the column dimensions are adjusted to handle the liquid and vapor provided by condenser and reboiler condition. The packing type is selected due to the availability in small size, and its size is selected to be small enough compared to the column diameter in order to prevent maldistribution of gas and liquid as well as providing high mass transfer efficiency due to high specific surface area.

Due to the dynamic nature of the batch distillation process, all details regarding the fluids' holdup volume and flow regime within the unit are highly influential on simulation accuracy. Also, the pressure profile is a decisive factor for a precise simulation since it affects the equilibrium and, subsequently, the process evolution. Moreover, for cases involving small feed quantities, such as in batch distillation, hydraulic considerations become more critical due to the relatively high ratio of holdup volume to feed quantity. Accordingly, the hydraulic calculations, including the pressure drop and flooding, are conducted using the Eckert model [26] to achieve an accurate prediction of the process.

The simulation is performed based on equilibrium stages, which is a reasonable assumption considering the small diameter of the column and packing size. Considering the equilibrium phase diagram shown in Fig. 1a, three phases of vapor–liquid-liquid (VLL), are defined and introduced to the simulation case using the UNIQUAC model.

A decanter is added to the unit downstream of the condenser as it is found to be an effective element in improving the heteroazeotropic batch distillation performance. Based on the simple decanter control approach described in a previous study [14], the liquid levels of $H_1 = 0.2m$ and $H_2 = 0.1m$ are set in the decanter to provide a perfect decanter condition. The term "return fraction," defined as the fraction of a condensed liquid phase returning to the column (along with the reflux stream), is applied to characterize the decanter performance. The

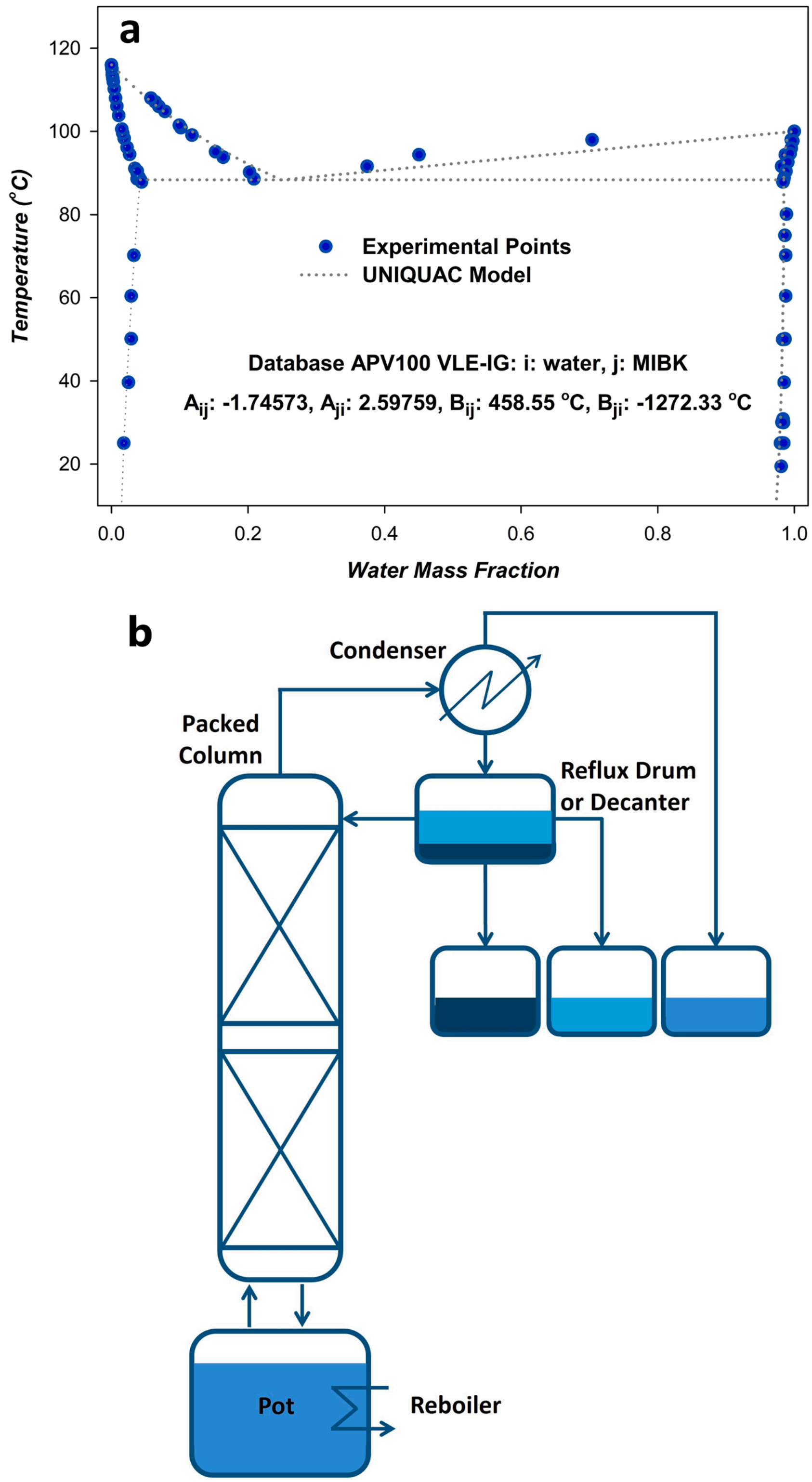

Fig. 1. (a) Phase equilibrium diagram of MIBK-water system at 1 atm and temperature range: 0–116 °C [24] (b) Schematic view of a conventional batch distillation unit.

relationship between return fraction, *RF*, and the well-known term reflux ratio, *RR*, is as follows:

$$RR = \frac{R}{D} \quad (1)$$

$$RF = \frac{R}{D+R} = \frac{RR}{1+RR} \quad (2)$$

where *D* and *R* are the mass flow rates of distillate and reflux streams, respectively. The return fraction value is bounded in the range $0-1$ in contrast with the reflux ratio that varies in the range $0 - \infty$, which makes it easier to understand and relate to the decanter separation performance (e.g., decanting efficiency of 90 % implies on $RF_1 = 0.9$ and $RF_2 = 0.1$).

Table 1
Geometrical and technical characteristics of simulated batch distillation unit.

Parameter	Symbol	Value/ Description	Units
Applied Module	–	*BatchSep*	$[-]$
Still volume	V_s	*120*	$[l]$
Diameter at condenser inlet	ϕ_c	*0.1*	$[m]$
No. of distillate collectors	–	*3*	$[-]$
Column section diameter	ϕ_s	*0.1*	$[m]$
Packing type	–	*Metal Raschig ring*	$[-]$
Packing size	ϕ_p	*1/2*	$[inch]$
Height of the equivalent theoretical plate	*HETP*	*1*	$[m]$
Packing Bed Height	H_p	*2*	$[m]$
Dry Packing factor	F_p	*984*	$[m^{-1}]$
Packing porosity	ε	*0.85*	$[-]$
Specific area of packing	α	*400*	$[m^2/m^3]$
Foaming (system) factor	f_f	*1*	$[-]$
Decanter diameter	ϕ_d	*0.1*	$[m]$
Decanter height	H_d	*0.4*	$[m]$

* Characteristic data for metal Raschig ring 1/2″ can be found in [25].

Table 2
Operating conditions and general process characteristics of simulated batch distillation process.

Parameter	Symbol	Value	Units
Feed quantity	r_0	*20–80*	$[kg]$
Feed temperature	$T_f = T_{f1}$	*25*	$[^\circ C]$
Product quantity (Recovered mass)	r	–	$[kg]$
Operating pressure (Condenser pressure)	$P = P_c$	*1*	$[atm]$
Initial MIBK mass fraction (Feed)	x_{r0}	*0.98*	$[-]$
Required MIBK mass fraction (Product)	x_r	*0.998*	$[-]$
Reboiler duty	W	*1200*	$[Watt]$
Condenser type	–	*Total*	$[-]$
Condenser outlet temperature	T_c	*85*	$[^\circ C]$
Decanter separation efficiency	η_d	*1*	$[-]$
Organic phase (MIBK-rich) level in decanter	H_1	*0.2*	$[m]$
Aqueous phase level in decanter	H_2	*0.1*	$[m]$
Organic phase (MIBK-rich) return fraction	RF_1	*1*	$[-]$
Aqueous phase return fraction	RF_2	*0*	$[-]$

The operation is defined by a constant reflux ratio for each phase, and simulation covers the operation in all steps of feeding, heat-up, and production until achieving the desired purity of 99.8 *wt.* % in the pot, defined as the simulation stop criteria. Based on the previous studies, the operation is simulated under the single-step operation (SSO) strategy, in which operation under total reflux condition as a start-up step is skipped, and the top outlet streams (distillate) are open from the beginning of the operation. The desired product, mainly comprised of MIBK, is collected in the pot, and the aqueous phase containing a slight amount of MIBK leaves the unit as the top product and is collected in a distillate collector. The initial condition of the simulated unit is as an empty unit, and the final condition is set to discharge the holdups of the column, condenser, and decanter to the distillate collectors. The potential top product mixture is divided into three streams: (1) MIBK-rich phase liquid, (2) aqueous phase collection, and (3) vapor phase collecting. In order to simulate the operation from feeding and heat-up steps, nitrogen gas is introduced to the model as "pad gas" to initially fill the column and containers.

The *state variables* applied to evaluate the operation performance of batch distillation include process time (t), fractional recovery (η), specific product flow (*SPF*), and specific energy cost (*SEC*) as defined by the following relationships [12,27]:

$$\eta = \left[\frac{r.x_r}{r_0.x_{r0}}\right] = \left[\frac{kg_{MIBKobtained}}{kg_{MIBKfed}}\right] \tag{3}$$

$$SPF = \left[\frac{r.x_r}{t}\right] = \left[\frac{kg_{MIBKobtained}}{h_{operation}}\right] \tag{4}$$

$$SEC = \left[\frac{W}{SPF}\right] = \left[\frac{kJ/h_{operation}}{kg_{MIBKobtained}/h_{operation}}\right] = \left[\frac{kJ}{kg_{MIBKobtained}}\right] \tag{5}$$

2.2. Unit configurations and operation policies

Different parameters such as unit configuration, operation policy, accessory elements, and control strategy significantly affect the batch distillation performance. Three configurations are studied in the present work, as illustrated in Fig. 2. The configuration, referred to as Mode I, is a conventional batch distillation unit equipped with a decanter. Mode II represents a unit with top feeding, commonly known as an inverted batch distillation unit, and Mode III is a unit with gradual feeding to the pot. The following sections provide a detailed description of the unit configurations and the operation scenarios. Different parameters, including feed quantity, feed stream position, and feed flow rate/feeding time, are studied. The detail of each assessment is presented in the following sections.

2.3. Effect of feed quantity – Mode I

As explained in section 2.1, the operation can be done with different feed amounts in the range of 20 to 80 kg. This limit depends on the still capacity and heating facilities of the unit. The holdup content in the column, condenser and decanter discharges at the end of operation, called "holdup loss", and its amount is almost constant, regardless of the feed quantity. Accordingly, processing a larger feed quantity at once is expected to lower the MIBK loss which consequently leads to a lower energy cost and a higher production rate. The feed quantity range of 20–80 kg is assessed in this part of the study to measure the impacts of feed quantity, and the relevant results are presented in section 3.1.

2.4. Top feeding (Inverted batch distillation) – Mode II

Typically, batch distillation units are initially fed in the pot, where the feed is heated during the operation. The configuration introduced as Mode II, is also known as inverted batch distillation or batch stripper [6,28,29], while the conventional batch distillation unit is known as a batch rectifier. This conveys the idea that Mode II can be applied to mixtures in which a small fraction of light components wants to be removed from heavy components, as in the MIBK-water mixture [30]. This configuration is also suggested for separation of mixtures with a minimum boiling azeotrope [31] and in cases for which the batch rectifier is not feasible [8]. The inverted batch distillation unit, modified by adding a decanter, has been previously applied for MIBK-water separation and proved to be an efficient method for upgrading the unit performance in terms of energy efficiency and production rate [14].

The feed tank in Mode II is located above the column and contains the feed mixture at 25 °C, which discharges to the column over the packing bed. The "feeding step" is defined and introduced to the model as the first step of the operation time schedule, in which the operation starts with the simultaneous commencement of feeding and pot heating. The feeding step finishes once the feed content is entirely discharged into the column. In the next steps, the feed stream is cut off, but the heating in the pot continues until the desired purity in the pot is achieved. The feed rate profile is specified by feeding time and the feeding scenario. Three different feeding scenarios are employed for Mode II (and Mode III), as described below:

1- Decreasing feed rate profile (gravity feeding): This scenario keeps the unit as simple as possible with no need for a fluid driver on the feed stream. It is assumed to discharge the feed mixture into the pot by opening the feed container discharge valve. The feed profile in this

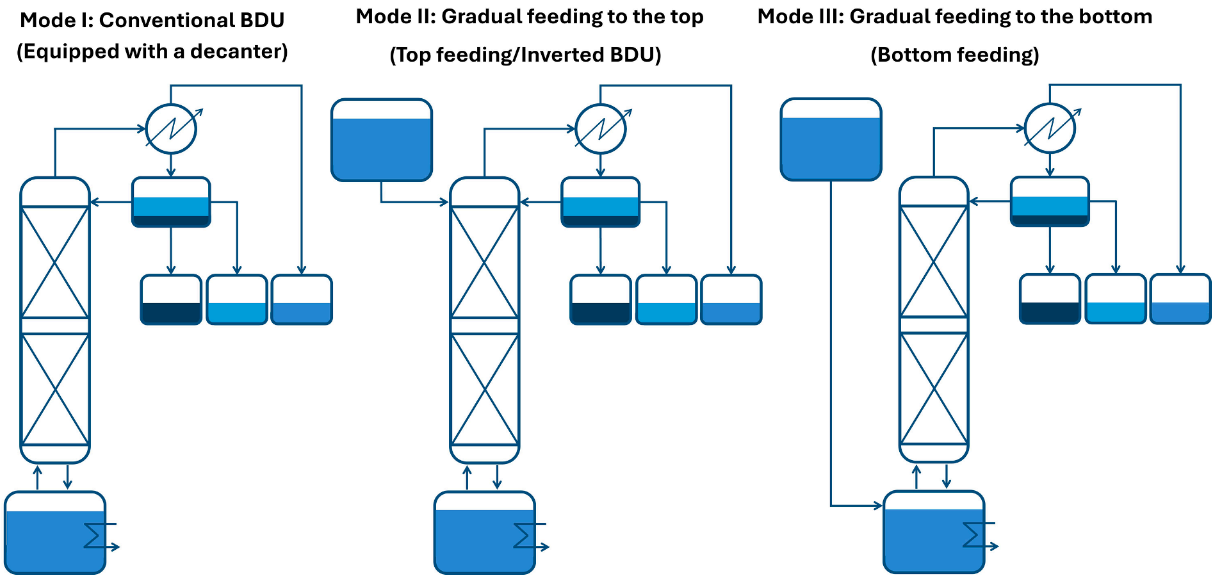

Fig. 2. Three studied batch distillation configurations.

scenario depends on the liquid level within the feed tank, and it is assumed to decline linearly during the time until the feed tank is drained completely. For a specified feeding time of t_f, the initial and final feed flow rate will be equal to:

$$F_0 = \frac{2r_0}{t_f} \quad (6)$$

$$F_t = 0 \quad (7)$$

where r_0 is the total feed quantity, and F_0 is the feed stream flow rate at the moment of opening the valve, located on the feed tank outlet nozzle. A ramping-down profile is adjusted for the feed flow rate, which varies from F_0 to $F_t = 0$ along the feeding step duration, t_f.

2- Fixed feed rate profile: This scenario is potentially easier for operation and evaluation, but it probably needs a fluid driver and a feed flowrate control system, which impose an extra cost. Accordingly, it should be studied and well justified before applying. The feed profile in this scenario is fixed, and for a specified feeding time of t_f, the initial and final feed flow rates will be equal to:

$$F_0 = F_t = \frac{r_0}{t_f} \quad (8)$$

3- Increasing feed rate profile: This scenario also needs a fluid driver and a controller to increase the feed flow rate gradually. For a specified feeding time of t_f, the initial and final feed flow rates will be equal to:

$$F_0 = 0 \quad (9)$$

$$F_t = \frac{2r_0}{t_f} \quad (10)$$

where r_0 is the total feed quantity and F_0 is the feed stream flow rate right before opening the valve located on the feed tank outlet nozzle. A ramping-up profile is adjusted for the feed flow rate, which varies from $F_0 = 0$ to F_t along the feeding step duration, t_f.

Applying these three feed profiles with various feeding times in Mode II, the production rate and energy index is specified, and the results are presented in section 3.2.

2.5. *Bottom feeding (Gradual feeding) – Mode III*

Applying an inverted batch distillation unit has been proven to be an efficient approach to upgrading the studied batch distillation process [14]. Two main factors are identified as contributing to the unit's performance improvement: (1) top feeding, which leads to the contact between the descending liquid and the rising vapor, and (2) gradual feeding, which leads to an earlier feed boiling. The contribution of each factor to performance improvement needs to be determined to provide deeper insight into the operation. Accordingly, gradual feeding to the bottom of the column (below the packing bed) is also evaluated. This configuration represents a case in which the feed container and reboiler are separated, while in a conventional batch distillation unit, these elements are combined and located at the bottom of the column. Similar to the top feeding strategy assessment (section 2.3), three different feed profiles with various feeding times are applied and evaluated in Mode III. The results obtained for operation under this strategy and the comparison of Mode II and Mode III are presented in section 3.2.

2.6. *Heat integration in a gradually fed BDU – Mode II*

As explained in the section. 1, the primary challenge for heat recovery in a batch distillation unit is the higher temperature of the pot or reboiler compared to the top vapor stream. This temperature difference precludes the effective use of conventional heat recovery methods or makes them economically infeasible due to high implementation costs. On the other hand, applying the gradual feeding operation policy transforms the batch process into a semi-continuous operation, in which the inlet stream with a remarkably lower temperature than the condenser has a great potential to receive the energy stream exiting the condenser. This opportunity enables us to employ the heat recovery techniques commonly implemented for continuous distillation. The first and simplest technique for heat recovery/integration is to employ a heat exchanger contacting the feed and the top vapor. Although this technique may be complex for theoretical evaluation or prediction, initial analysis and energy balance checks suggest that it can potentially (1) reduce condenser utility consumption and (2) intensify the process and accelerate the operation rate by preheating the feed, which implies higher input energy to the unit. The results and more details on heat recovery are provided in section 3.3.

3. Results and discussion

Batch operations might be performed and analyzed under two different perspectives of *single batch* and *sequential batches*. The former applies for the cases with only one time operation and the latter is applicable for the cases in which the process repeats frequently and subsequently provides a higher production capacity in the course of time. Depending on the frequency of operation and the subsequent applied perspective, different state variables should be employed to assess the operation. The evaluation of a batch unit operation in this study is done based in *sequential batches* perspective. Based on this perspective, the suitable criteria for performance evaluation are the *SEC* and *SPF*. Also, some state indexes are defined, enabling us to present the results concisely and more illustratively. These state indexes applied to present the fractional recovery, η, specific energy cost, *SEC*, and specific product flow, *SPF*, are calculated as follows [13,14]:

$$\text{Recovery Index } \eta_i = \left[\frac{\eta}{\eta_d}\right] \tag{11}$$

$$\text{Production rate index}: \quad P_i = \left[\frac{SPF}{SPF_d}\right] \tag{12}$$

$$\text{Energy cost index } E_i = \left[\frac{SEC_d}{SEC}\right] \tag{13}$$

The letter 'd' represents the reference case, which is the case with a feed quantity of $r_0 = 80\ kg$ processed in Mode I. The state variables obtained from this case are presented in Table 3, and the associated state indexes are equal to 1. The higher value of state indexes implies a more favorable operation, and the values larger than 1 show the superior performance of an operation over the reference case. On the other hand, the indexes below 1 indicate a relatively unfavorable case compared to the reference case. It is worth mentioning that due to the relationship between the *SPF* and *SEC* in this study ($SEC \times SPF = W = Const.$) the relevant indexes (Eq. (12) & (13) are identical, so applying only one index is sufficient for both.

3.1. Effects of feed quantity − Mode I

As explained in section 2.3 and considering the pot volume, different feed quantities in the range 20 to 80 kg are evaluated. Fig. 3 indicates the state indexes obtained in each case. As this graph shows, increasing the feed quantity leads to a higher recovery index as well as a higher production rate and energy index, so increasing the feed mass from 20 to 80 kg results in over 4 % improvement in all state indexes. This can be explained by the smaller fraction of "holdup loss" in operations with larger feed quantities compared to multiple operations with smaller feed amount. Accordingly, the feed quantity of 80 kg is employed in the rest of this study.

3.2. Gradual feeding strategy − Mode II and Mode III

Based on the operation time obtained in Mode I for processing an 80 kg feed mixture (402 min.), the feeding time in the range of 0 to 390 min is selected for gradual feeding assessment. Different feeding times are applied to three feeding scenarios: decreasing feed rate, fixed feed rate, and increasing feed rate to assess the impact of the feeding schedule (time and profile) on the unit performance and state variables. The values of production rate and energy index obtained at different feeding schedules are shown in Fig. 4. The point $t_f = 0$ on the x-axis corresponds to the operation in Mode I, in which the feed is already charged in the pot. As this figure shows, the short feeding times (below 120 min) in Mode II and Mode III change the state index (production rate and energy index) very slightly, and it is almost equivalent to Mode I. By extending the feeding time, the differences become more significant, and each feeding schedule shows a unique behavior. Overall, Mode II (top feeding) offers a more efficient operation in all cases compared to Mode III (bottom feeding) for the same feeding schedule. The results obtained for three feeding profiles are explained below:

1- The increasing feed rate profile causes adverse changes in the state index for both Mode II and Mode III, so it is not a potentially suitable feed profile.
2- The fixed feed profile in Mode III (bottom feeding) results in adverse changes in state index, and its effect becomes more significant with extending the feeding time, while the same feeding profile in Mode II (top feeding) results in a higher state index. The maximum state index of 1.06 is obtained at a feeding time of 300 min, and extending the feeding time beyond this point leads to a decline in the production rate and energy index.
3- The decreasing feed rate profile in Mode III (bottom feeding) does not change the process significantly, and the results are almost the same as Mode I, while it favors the state index in Mode II (top feeding) by extending the feeding time up to 360 min, at which the maximum state index is obtained. At this point, the total operation time is 365 min, which means the operation takes only 5 min longer than the feeding, and it is very close to a continuous operation. The state index of 1.10 shows a 10 % improvement in energy efficiency and production rate at this point. Beyond this point, the mixture reaches the desired purity before the end of the feeding stage, so the feeding time determines the total operation time.

In the previous work [14], two main mechanisms were identified as influencing separation performance in a gradual feeding scenario in Mode II: (1) the earlier boiling of the feed, implying a shorter start-up and quicker onset of production, and (2) the presence of a descending liquid flow in top-feeding configuration, which drives the mass transfer (stripping) within the column. The former highlights the impact of gradual feeding, while the latter emphasizes the effect of feeding location (top/bottom). Accordingly, superior performance of the top feeding scenario (Mode II) over the bottom feeding scenario can be explained by the impact of vapor–liquid contact provided through introducing a downward liquid feed stream to the column section, which favors the intended stripping process (MIBK dehydration) in contact with the rising vapor flow provided shortly after the operation begins. Further details on the governing mechanism and explanations for these observations are provided in Section 3.3.

3.3. Heat recovery − Mode II and Mode III

As explained in section 3.2, top feeding (Mode II) is potentially a more effective approach compared to conventional feeding policy (Mode I) under a proper feeding profile, while bottom feeding (Mode III) is almost equal to or less efficient than Mode I. Regardless of these differences, both of the so-called "gradual feeding" scenarios (Mode II and Mode III) enable us to easily apply any well-developed heat recovery approach on a batch distillation unit and upgrade its energy efficiency.

Fig. 5 illustrates a simple configuration that enables the recovery of heat from the top vapor stream to the feed stream. In this configuration, two condensers (HEX I and HEX-II) are employed. In the first one (HEX-I), which can also be referred to as a heat recovery exchanger or a feed preheater, the feed stream serves as a coolant. Due to the limits in the

Table 3
State variables obtained in the reference case (Mode I with feed quantity of $r_0 = 80\,kg$).

State variable	Symbol	Value	Units
Process time	t_d	402	$[minute]$
MIBK Recovery	η_d	98.86	$[\%]$
Specific Energy Cost	SEC_d	369.2	$[kJ/kg]$
Specific Production Flow	SPF_d	11.70	$[kg/h]$

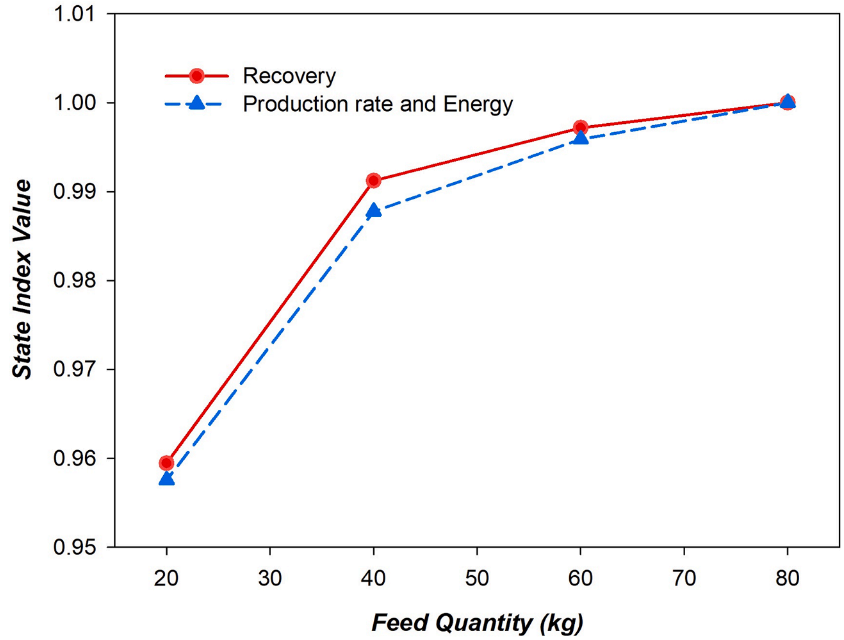

Fig. 3. Effects of feed quantity on state indexes.

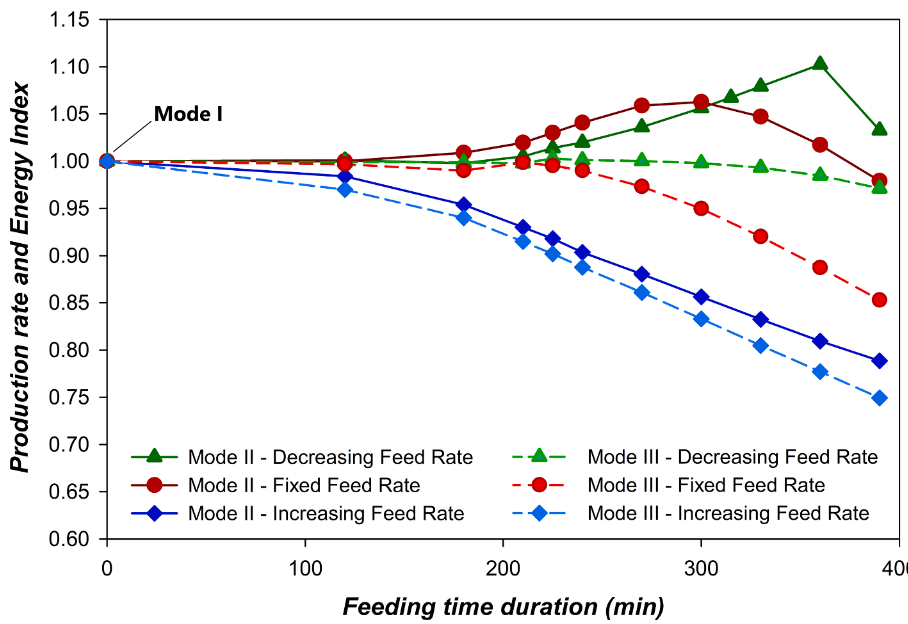

Fig. 4. Effect of feeding time duration on distillation performance in Mode II (top feeding) and Mode III (bottom feeding).

dynamic batch distillation module (BatchSep) provided by Aspen Plus, the proposed heat recovery configuration cannot be defined in simulations, but a fraction of the heat stream leaving the distillation column condenser is transferred to the inlet feed stream by adding a heater block to the flowsheet. Hence, the following assumptions are made to simplify the assessment and keep the solution consistent with the real case:

1- The feed stream (F-MII) can be heated up to 85 °C (below the bubble point at the azeotropic composition) and boiling in the feed stream does not take place. There is certainly potential for boiling in some cases, which may intensify the process beyond the predictions in this study. However, it is preferable to underestimate the potential of the proposed approach rather than overestimate it.

2- The condenser outlet temperature (HEX-II) is fixed to 85 °C. Accordingly, considering the condenser as a preheater with a hot stream outlet temperature of 85 °C, heating a cold stream to 85 °C is not a critical task, and it can be done by employing a simple and small heat exchanger, which also ensures the viability and low capital cost of the proposed solution.

3- Reboiler duty and condenser outlet temperature (HEX-II) are equal to the previously studied cases (Table 2). Heat recovery serves as a process intensification approach, requiring minor modifications and simple control systems in the unit.

4- Based on assumptions 2 and 3, the heat transfer/recovery to the feed begins a few seconds after initiating the condensation in the condenser. The heat recovery gradually increases the feed

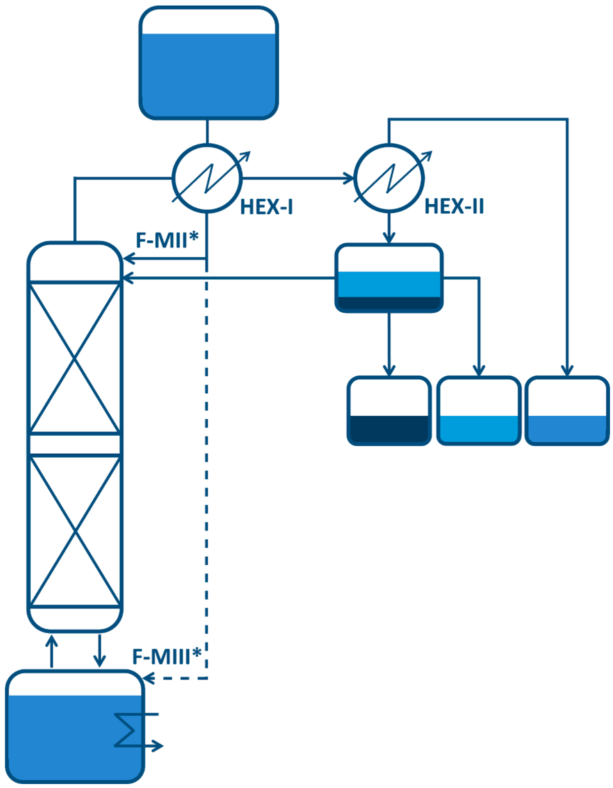

Fig. 5. Proposed configuration for heat recovery from top vapor to the feed stream in a batch distillation unit operating under gradual feeding scenario (Mode II / Mode III).* Feed streams, F-MII and F-MIII, correspond to Mode II and Mode III, respectively.

temperature to 85°C by 10 min, and it remains fixed until the end of the feeding step.

According to these assumptions, the estimation of heat recovery potential in this study is conservative and it is possibly higher in real cases compared to the results provided in this study. Before addressing heat recovery, a primary evaluation is conducted on the potential of heat recovery and subsequent operation enhancement through theoretical discussion. To this end, the condenser heat duty profile during the process is compared to the inlet feed heat absorption potential, that is calculated as the maximum enthalpy change that can undergo when changing its temperature from T_{f1} and T_{f2}, which are the feed temperature upstream and downstream of the heat recovery exchanger, equal to 25°C and 85°C, respectively. Accordingly, the instant heat recovery to the feed stream, dQ, is determined as follows:

$$dQ = FC_p(T_{f2} - T_{f1})dt \quad (14)$$

where, F is the feed mass flow rate, C_p is the feed mixture specific heat capacity and t is time . Integrating this relationship over the process time results in the accumulative potential capacity of heat recovery by feed stream, Q.

Fig. 6 presents the temporal variation of condenser heat duty and the estimated heat recovery potential of the feed stream for Mode II and Mode III at the same feeding time (300 min). As this figure shows, the condensation starting time depends on the feed rate profile (increasing, decreasing, or fixed rate) and the feeding location (top or bottom). The condenser heat duty and the feed heat recovery potential follow the same trend in Mode II and Mode III, and there are only minor differences between the two configurations. On the other hand, different feed profiles lead to distinctly different unit behaviors, highlighting the significant impact of the feed rate profile. These observations align with Fig. 4 and the discussions in Section 3.2. According to Fig. 6, the condenser heat duty and the heat recovery potential, which are equal to zero before a specific time, start rising as soon as the vapor reaches the condenser. The condenser heat duty profile reflects the dynamic behavior of vaporization in the reboiler and condensation in the condenser.

Comparing different feeding locations (Mode III vs. Mode II), condensation begins sooner in Mode III (bottom feeding) than in Mode II (top feeding). Also, the condenser duty increases gradually in Mode III while it rises sharply in Mode II. This ramping trend gains importance in the feed stream temperature rising time since the heat transfer to the feed cannot exceed the condenser heat duty. In the present study, a 10-minute period for raising the feed stream temperature has been adjusted based on this limitation (assumption no. 4, section 3.3). Comparing different feeding profiles (increasing, decreasing, or fixed feed rate)

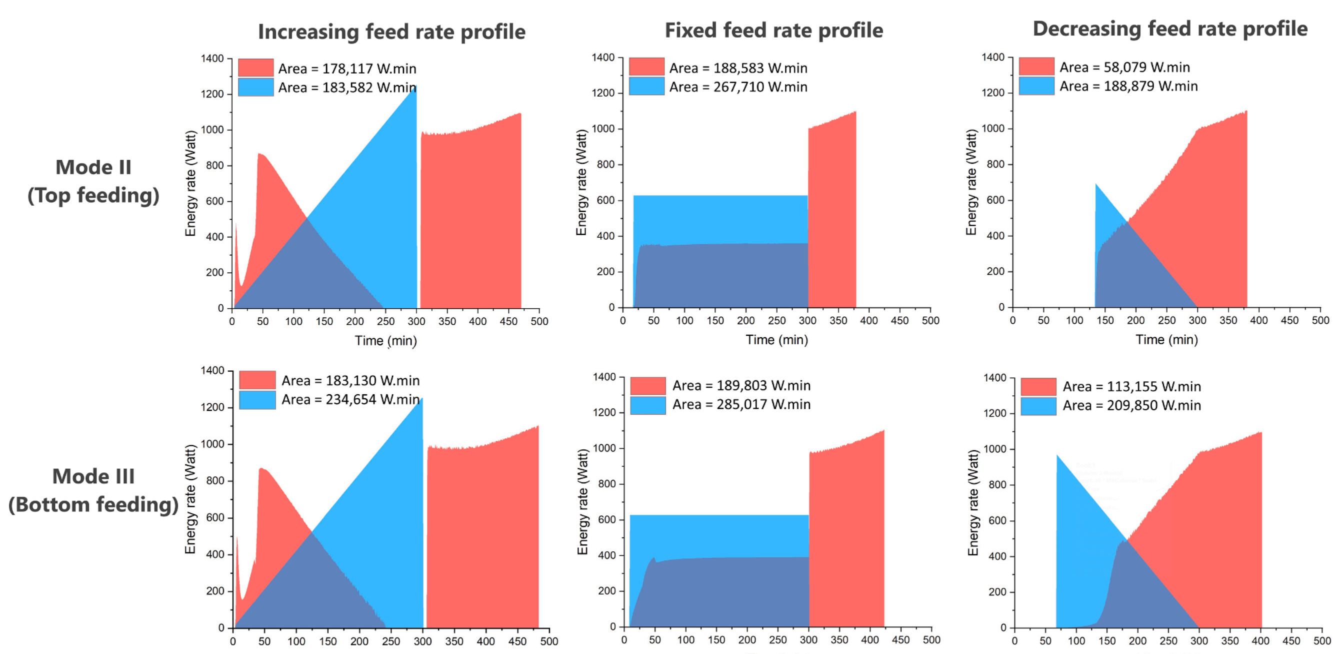

Fig. 6. Condenser heat duty and feed stream heat recovery potential in Mode II and Mode III under different feed profiles.

shows that boiling and condensation start sooner for an increasing feed flowrate, followed by the fixed feed flowrate and the decreasing feed flowrate, respectively.

Despite the earlier boiling and condensation in Mode III, which implies a shorter start-up and earlier production, it results in a longer operation time compared to Mode II (see section 3.2). Also, despite the shorter start-up period by applying an increasing feed rate profile (in both Mode III and Mode II), it results in a longer operation time (see section 3.2) and the lowest state indexes compared to other feed rate profiles (even lower than Mode I). The undesirable results obtained from a top feeding configuration (Mode III) with an increasing feed rate profile indicate that the suitable feeding location and early boiling/condensation initiation (shorter start-up period) do not necessarily guarantee a desired operation. This suggests that there is a third factor influencing the operation: the stability of operation and quality of liquid–vapor contact within the column. This stability is defined by uninterrupted vapor and liquid streams with well-balanced flow rates, ensuring neither dominates each other nor disrupts the process. Maintaining these conditions creates a favorable hydraulic environment, preventing issues such as flooding, dry stages, choking, or suppressed boiling in the pot. In other words, consistent vapor and liquid streams with properly balanced flow rates is the key to efficient operation and desirable results. Accordingly, the unfavorable performance of Mode II (top feeding) with an increasing feed rate can be attributed to interrupted boiling and condensation, as illustrated in Fig. 6. The results for the three feeding profiles are outlined below:

- For the increasing feed rate profile, boiling and condensation take place soon after starting the operation, which is due to the small content of the mixture within the unit. As explained, having a shorter start-up period in this case does not lead to a desirable result, and it offers the lowest state indexes compared to other studied operation policies. As shown in Fig. 6, the condenser heat duty starts growing sharply and then declines drastically in the first few minutes of operation. The initial sharp rise can be attributed to the small content of feed mixture vaporized immediately by reboiler, and the sharp decline is due to entering a growing rate of low-temperature liquid feed, which cools down the unit content and dampens the boiling. By further heating in the pot, the boiling intensifies again, leading to a second rise in condenser heat duty, which continues for about 15 min but diminishes again down to 0, which persists until the end of the feeding stage. This is also due to introducing a greater amount of low-temperature liquid feed into the unit, which lowers the pot content temperature and halts boiling. The growing rate of liquid and the unstable vapor rate yield in a poorly balanced flow rate of liquid and vapor, an improper vapor–liquid contact within the column (implying a poor hydraulic condition), and ultimately leads to pausing the vapor generation by quenching the pot content. Also, the production is halted in a large fraction of the feeding period, and the operation after this period does not leverage any downward liquid flow in the column section, which is similar to operation in Mode I. Accordingly, the production stage takes place initially for a short period, then it halts until the end of the feeding period, and it continues with the same principles as in Mode I. Overall, this condition resembles an interrupted operation in Mode I, and it explains why an increasing feed rate profile results in state indexes lower than Mode I. Since the interruption is basically due to entering low-temperature liquid, applying heat recovery and increasing the feed stream temperature may potentially prevent the interruption in process and accelerate the operation. The higher condenser duty compared to the feed stream heat recovery capacity at the start of the production step ensures the heat recovery potential, while after a particular time, the heat rate required to increase the feed temperature to 85 °C (based on assumption no. 1) exceeds the condenser duty, which is not consistent with the heat recovery principle. This can be predicted by observing the rising profile of the feed stream heat recovery potential in Fig. 6. In addition, the increasing feed rate, along with the boosted liquid and vapor rate induced by heat recovery, can further complicate the hydraulic conditions, escalate the risk of extreme scenarios such as flooding, and complicate the process control.
- For the fixed feed rate, the boiling and condensation start time is shorter than the decreasing feed profile and longer than the increasing feed profile. The feed heat recovery potential and the condenser duty remain constant until the end of the feeding stage. Immediately after the feed stream is cut off, a drastic rise in condenser heat duty can be observed. This is because the liquid feed entering the unit mitigates the boiling during the feeding phase, which lowers the vapor reaching the condenser and, subsequently, the heat duty of the condenser. These values rise sharply by cutting off the feed stream. These observations indicate that while the gradual feeding at a fixed flow rate improves the production rate and energy cost (at least in Mode II), it defers a large fraction of condenser thermal load to the end of the operation. Since this amount of heat load does not coincide with the feeding stage, it may seem out of reach for recovery by feed stream. Nevertheless, the heat recovery will intensify the process, reduce the process time, and escalate the condenser heat duty. Accordingly, an intensified process would take a shorter time after the feeding stage, and the peak heat duty at the end of the operation will be shifted to the left, where it can be recovered by feed stream. Based on this explanation, a fixed-flow feed stream has a high potential for heat recovery.
- For the decreasing feed rate profile, the heat recovery capacity of the feed stream declines linearly until it reaches $dQ = 0$ by finishing the feeding stage. Due to the relatively long delay in starting the boiling and condensation and the higher flow rate of the feed stream at first, a large fraction of feed enters the column before observing any boiling or condensation, so it loses the potential of feed for heat recovery, and considering the limit of 85 °C for feed temperature and excluding the boiling in the feed stream, the remained feed content has a low potential for heat recovery. Hence, despite the superior performance of the unit under a decreasing feed profile, this feeding profile is probably not the ideal case for heat integration.

Given that feed preheating (introducing a higher temperature feed) and condenser heat duty are interdependent and changes in one directly impact the other, heat recovery is expected to elevate the condenser duty and influence the overall operation trend. In other words, a preheated feed stream (higher temperature feed) intensifies the boiling rate in the pot, which in turn leads to an increased condenser duty. Accordingly, transferring heat from the condenser outlet to the inlet feed stream initiates a complex cascade of effects.

As explained, Fig. 6 is applied to partially explain the observations in section 3.2 and assess the feasibility of heat recovery in each scenario by comparing the heat duty of the condenser and the heat absorption potential of the feed stream. Due to the higher duty of the condenser compared to the estimated potential of feed stream heat recovery capacity, higher feed temperature and partial vaporization of feed are also possibly achievable in some cases (e.g., in decreasing feed rate profile).

Since the performance of Mode II (top feeding) is considerably higher than Mode III in this study, the heat recovery scenario is only applied to Mode II to achieve the maximum potential of introduced solutions for upgrading the batch distillation operation. Also, according to the insights gained from Fig. 6, a fixed-rate feed stream shows a great potential for heat recovery and a decreasing feed rate profile provides the highest state indexes. Accordingly, these two feed profiles are applied in Mode II for the further steps in heat recovery evaluations.

Fig. 7 demonstrates the energy and production rate index for Mode II (top feeding) with and without heat recovery implementation. Two feeding profiles of decreasing feed rate and fixed feed rate are evaluated. According to this graph, the fixed feed flow rate is a more efficient option for heat recovery as it can improve the production rate and energy index by 47 %, while employing the decreasing feed rate profile, the

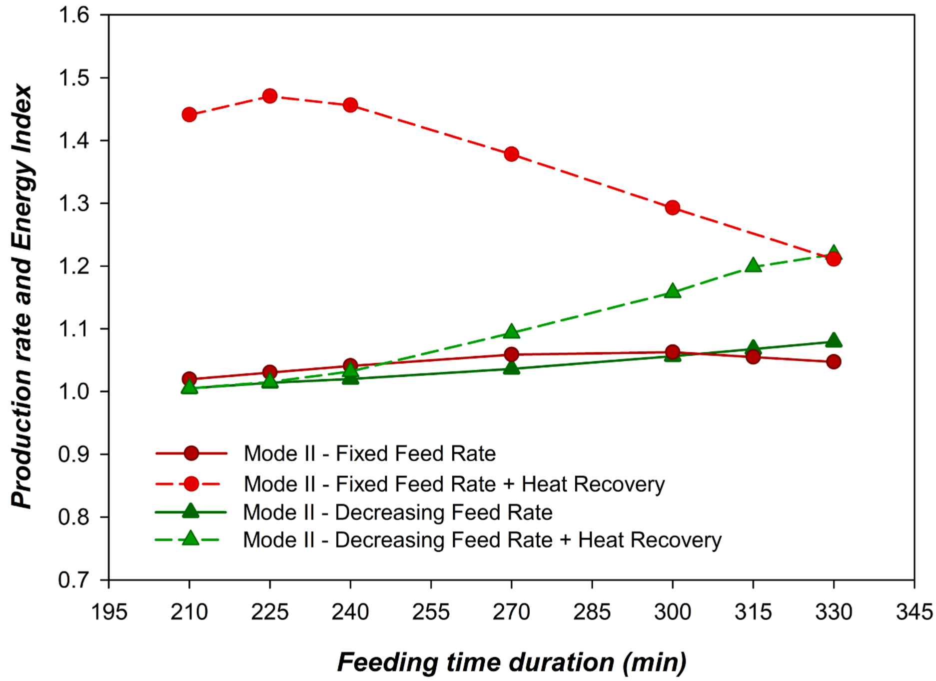

Fig. 7. Effect of heat recovery on Mode II (top feeding) with decreasing feed rate and fixed feed rate profiles.

maximum achievable improvement is about 22 %.

The range of 210 to 330 min for decreasing feed profile is selected because, with the feeding times shorter than 210 min, the boiling/condensation starts shortly before or after feeding termination, so transferring the condenser heat outlet to the feed stream feed is impossible. Additionally, if the feeding time exceeds 330 min, the desired purity will be achieved before the end of the feeding stage; thereby, the feeding time will be the controlling factor, which adversely impacts the production rate and the energy index. On the other hand, the range of 210 to 330 min for a fixed feed rate is selected because, with the feeding times shorter than 210 min, the required heat duty for heating up the feed to 85 °C exceeds the condenser heat duty during the operation, so it is not consistent with the principles of heat recovery and the assumptions of this study. Extending the time beyond 330 min does not enhance the process further, as the graph shows a decline as the feeding time increases.

4. Outlook on the future

By harnessing gradual feeding as an effective approach to improve batch distillation energy efficiency, different options become available for heat recovery. In addition to the proposed configuration in Fig. 5,

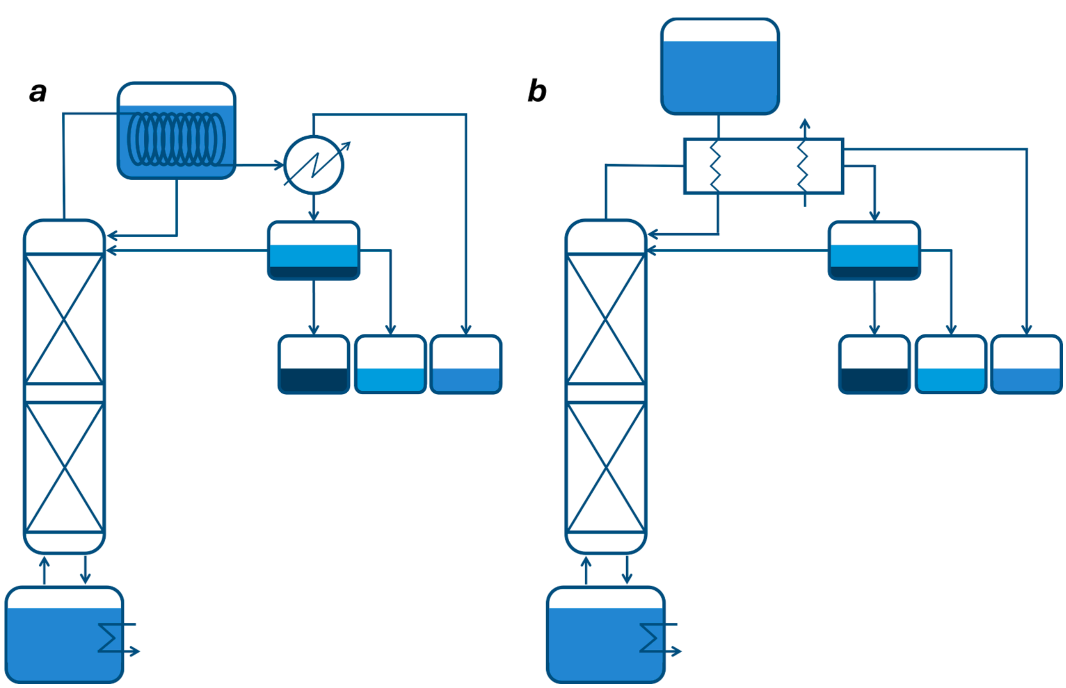

Fig. 8. Simple alternative configurations proposed for heat recovery from top vapor to the feed.

some other configurations can potentially be applied under a gradual feeding scenario, such as the one shown in Fig. 8a. In this configuration, instead of installing a heat exchanger for contacting the top vapor and the feed stream, the top vapor passes through a coil embedded inside the feed tank. Also, as shown in Fig. 8b, a specially designed heat exchanger with more than one coolant stream [32] can be applied instead of two condensers proposed in Fig. 5, or a heat pump can be applied to recover energy as much as possible [20]. These ideas or any other potential solution must be assessed in detail in further studies. Also, the heat energy profiles showed that an increasing feed flow rate profile leads to a shorter heat-up step. In this case, boiling initiates earlier, making heat recovery possible from the very first minutes of operation. On the other hand, a fixed feed rate has more potential for overall heat recovery, and it facilitates operation control. Hence, a combination of these approaches is probably ideal. In this scenario, the feed stream enters the unit with a ramping-up flow rate and, after a specific time, continues at a fixed rate until the end of the operation. These scenarios can be studied in further studies, along with other heat recovery approaches already developed for continuous distillation.

5. Conclusion

Batch distillation is applied for the dehydration of MIBK, which forms a heteroazeotrope with water. Three different unit configurations are evaluated in terms of production rate and energy efficiency. The main conclusions of the study on the conventional unit equipped with a decanter, Mode I, are outlined as follows:

- Evaluating the process by Mode I for different feed quantities in the range 20 to 80 kg shows that the larger feed quantity results in better unit performance, so the production rate and energy cost for 80 kg feed are around 4 % better than the case with 20 kg feed. This is explained by almost constant “holdup loss” regardless of the feed quantity, which leads to a lower fraction of loss to feed in cases with a larger feed quantity.

The evaluation of batch distillation unit with gradual feeding, Mode II (top feeding), and Mode III (bottom feeding), and comparing them to Mode I revealed that:

- The top feeding approach (Mode II) is found to be a more efficient approach compared to Mode III for separation of MIBK-water binary system by offering a higher production rate and energy index in almost all studied cases.
- All feed rate profiles provide very slight differences from Mode I for feeding time below 120 min (high feeding rate), and the differences become more tangible with the longer feeding times.
- The decreasing feed rate profile in Mode II offers up to 10 % enhancement in state index, while in Mode III it results in very slight changes.
- The fixed feed rate in Mode II can provide up to 7 % improvement in state index, while in Mode III results in adverse changes.
- The increasing feed rate profile in both Mode II and Mode III results in an equal or lower state index than Mode I, and its impact aggravates with extending the feeding time.
- Three main factors are identified as contributing to the effectiveness of the gradual feeding approach: (1) boiling commencement time, (2) feeding location, and (3) the quality and quantity of vapor–liquid contact within the column. The feed flow rate and profile determine these three factors in cases with constant reboiler duty.

Based on these results, the gradual feeding approach can serve as an effective method for upgrading a batch distillation unit by employing a proper feeding schedule (time and rate profile) and location. On the other hand, the temperature difference between the feed stream and the top vapor exiting the column in a gradual feeding scenario (Mode II or Mode III) provides a significant opportunity for heat recovery/process intensification. Leveraging this opportunity, the condenser outlet heat energy is transferred to the feed stream, heating it to 85 °C. The results for heat recovery potential assessment are outlined as follows:

- In case of implementing heat recovery, a fixed feed flow rate offers superior performance over a decreasing feed rate.
- The proposed heat recovery approach in Mode II with a fixed feed rate offers up to 47 % improvement in energy efficiency and production rate compared to Mode I, while the maximum achieved improvement with a decreasing feed rate profile is 22 %.

These findings indicate that the gradual feeding policy can transform the technical and economic framework in many applications of batch distillation via unlocking the heat recovery viability.

CRediT authorship contribution statement

Saber Niazi: Conceptualization, Investigation, Methodology, Formal analysis, Writing – original draft, Writing – review & editing. **José Antonio Díaz-López:** Conceptualization, Formal analysis, Supervision, Validation, Writing – review & editing. **Antonio Nieto-Márquez:** Conceptualization, Formal analysis, Supervision, Validation, Writing – review & editing, Project administration, Funding acquisition.

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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Data availability

Data will be made available on request.

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