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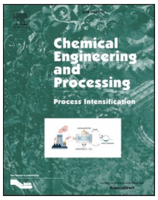

Are process-intensified extractive distillation always energetically more efficient?

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ABSTRACT

The thermally coupled, dividing wall column, and side-stream configurations are some of the energy-intensified techniques widely applied to the extractive distillation for improving the energy efficiency. Today, several heuristics are available for analysing the energy-saving efficiency of these intensified techniques for ideal distillation system but there is no heuristic available for analysing the complex distillations system. Therefore, it has not yet been established what variables affect the energy-savings and under what particular conditions the intensified processes for these complex distillation systems present energy-savings. In this work, we aim to provide insights and preliminary conclusions that open a field of study for a more detailed and in-depth analysis for future researches through three different case studies where their corresponding intensified configurations do not provide any energy-saving relative to the conventional extractive distillation (CED). Based on our preliminary analysis, we attributed this to the poor values of interconnecting flowrate or composition and high column internal vapour flowrate. Our results also revealed the possibility of extending several heuristics, previously developed for evaluating the energy-saving efficiency in ideal distillation system, for complex distillation. Lastly, several recommendations are given that were derived from our simulation results and the analyses we carried out on existing publications.

1. Introduction

Distillation-based process is a mature and well-researched unit operation that accounts for about 90% of all the separations [1]. In addition, it consumed about 50% of the energy in the chemical and refining industries and enables some of the world's largest and most profitable separations, e.g. crude oil fractionation, hydrocarbon separation, and natural gas liquids (NGL) separation. Among the many different well-established distillation-based processes, the conventional extractive distillation (CED) can be used for the separation of azeotropic mixture by relying on the introduction of an additional solvent (i.e. entrainer) into the system (i.e. mixture) to increase the relative volatility and alter the vapour-liquid equilibrium data in the azeotropic mixture [2]. Besides CED, the pressure swing distillation (PSD) can be used to separate azeotropic mixture, which presents the advantage of not requiring an additional solvent (i.e. entrainer). However, the application of PSD is limited to the separation of pressure-sensitive azeotropic mixture only, whose azeotrope composition changes significantly with pressure [3]. Other than using the aforementioned processes, some other distillation-based processes are also available such as the recently emerging membrane-assisted (pervaporation process) distillation (MD) [4] and hybrid reactive-extractive distillation (RED) for azeotropic separation [5]. However, majority of these distillation-based processes may have distinct operational costs, which generally comprise two major aspects, i.e. the total reboilers vapour duty requirement and the temperature level at which the vapour is generated and/or condensed [6]. The reboiler vapour duty is associated with the first-law of thermodynamic (i.e. heat duty requirement) while the temperature level correlates with the heating and cooling utility costs required for all the reboilers and condensers (i.e. second-law of thermodynamic). Following this, energy-saving is one of the important criteria that should not be omitted in distillation system design.

To date, several energy-intensified distillation techniques have been

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Abbreviations: PSO, particle swarm optimisation.

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Nomenclature

Abbreviations

CED	conventional extractive distillation
DCRED	double column reactive-extractive distillation
DMSO	dimethyl sulfoxide
DW-DCRED	dividing-wall double column reactive-extractive distillation
EDC	extractive distillation column
EDWC	extractive dividing wall column
EG	ethylene glycol
EO	ethylene oxide
ESI	ease of separation index
IV	vapour interconnection stream
IL	liquid interconnection stream
MD	membrane-assisted distillation
MINLP	mixed integer nonlinear programming
NGL	natural gas liquids
PSD	pressure swing distillation
RED	reactive-extractive distillation
REDC	reactive-extractive distillation column
SSED	side-stream extractive distillation
SS-DCRED	side-stream double column reactive-extractive distillation
SRC	solvent recovery column
TCDS	thermally coupled distillation columns
TCED	thermally coupled extractive distillation
TC-DCRED	thermally coupled double column reactive-extractive distillation
TAC	total annual cost
TBA	tertiary butyl alcohol
THF	tetrahydrofuran

devised such as the thermally coupled extractive distillation (TCED) [7], extractive dividing wall column (EDWC) [8], and side-stream extractive distillation (SSED) [9] for the separation of binary [10–12] and ternary azeotropic mixtures [13–15]; with each technique having several different configurations and its own characteristic. Generally, these energy-intensified techniques eliminate the remixing effect occurred in the conventional distillation and typically reduce the energy consumption up to 30% [16–19]. However, different configuration for a given technique may provide different energy-saving efficiency (e.g. the thermally coupled configuration with side-rectifier and side-stripper can have different energy-saving efficiency) (Fig. 1). Thus, one cannot be certain whether a particular configuration (e.g. thermally coupled with side-rectifier) is more thermodynamically efficient than the other (e.g. thermally coupled with side-stripper), unless exergy analysis is carried out [6]. For example, Finn [20] worked on the separation of propane, i-butane, and n-butane using thermally coupled configuration with side-rectifier and direct split. They showed that although there is a significant reduction in the total heating duty in the case of side-rectifier configuration, such benefit however was traded-off at an expense of an increase in the actual work requirement in comparison to the direct split configuration.

Our literature survey has indicated that all the existing studies on the intensified extractive distillation always use the total annual cost (TAC) as their main objective [21–24], with a handful number of multi-objective optimisation studies considering some other secondary objectives such as environmental (e.g. CO_2 emissions), inherent safety, and dynamic controllability [25–28]. Nevertheless, it is worth highlighting that no existing studies had analysed which of the corresponding energy-intensified configuration provides the best energy-saving, what are the variables that affect the energy-savings, and under what particular conditions the energy-savings do not occur for complex (e.g. extractive) distillation system. Note that although most of the existing studies have reported that the energy-intensified processes can provide significant energy-savings, our literature survey has found three recent studies reported in literature where the energy-intensified processes cannot provide any energy-saving in comparison to the CED, contrary to most of the existing studies. The first study is the work of Yang et al. [29] on the ternary azeotropic separation of tertiary butyl alcohol (TBA), ethanol, and water. Although they reported that the dividing wall double column reactive-extractive distillation (DW-DCRED) provides the lowest TAC and CO_2 emission, the energy consumption is higher, by marginal, in comparison to the double column reactive-extractive distillation (DCRED). The second study is from the work of Zhao et al. [30] that evaluated the separation of tetrahydrofuran (THF), ethanol, and water. They investigated two different TCED configurations using mixed entrainer (i.e. 60 mol. % dimethyl sulfoxide (DMSO) + 40 mol. % ethylene glycol (EG)), i.e. the first configuration connects the first and second extractive distillation columns (EDCs) (i.e. EDC 1 and EDC 2) while the second configuration links the second and third distillation columns (i.e. EDC 2 and solvent

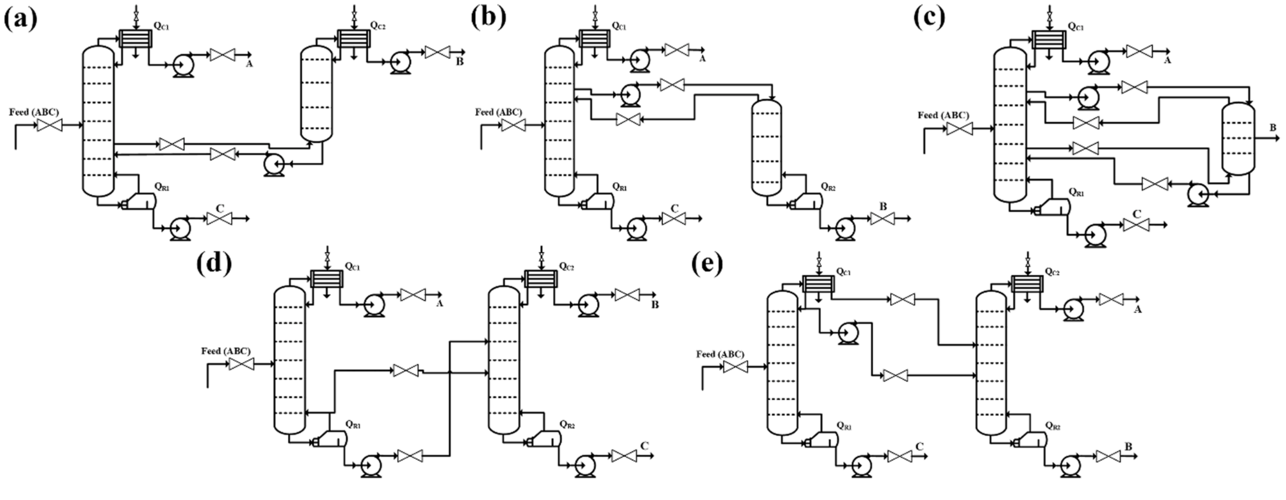

Fig. 1. Thermally coupled distillation column for ternary separation with (a) side-rectifier, (b) side-stripper, (c) fully thermally coupled (i.e. Petlyuk configuration), (d) direct-split, and (e) indirect-split.

recovery column (SRC)). The second TCED configuration does not provide any energy-saving relative to the CED. The most recent study is the work of Liu et al. [26] on the separation of ethyl-acetate, ethanol, and water. They indirectly showed that the energy of the intensified DW-DCRED is higher than the DCRED by about 3%, despite having a lower TAC by about 8.16%. Upon analysing the results from these three studies [26,29,30], it becomes apparent that the energy-intensified processes (e.g. thermally coupled or dividing wall) do not provide any energy-saving relative to the CED. In essence, these three studies had indirectly demonstrated that the energy-intensified processes do not always contribute towards significant energy-savings [26,29,30]. To date, our literature survey has indicated that there are no existing studies that explain why these energy-intensified processes could not provide any energy-savings relative to the CED for the separation of azeotropic mixture.

On the other hand, significant progress has been made towards evaluating and comparing the energy-efficiency of the different configurations under the same intensified technique for ideal distillation system [31–38]. Several literatures had provided comprehensive discussion on the different configurations for the thermally coupled and dividing wall for ideal distillation system, which can be referred to [39–41]. Other than that, several studies had, for example, modified and applied the well-established Underwood's classical method to analyse the energy-saving efficiency in dividing wall [42–47] and thermally coupled configuration [6,48] for ideal distillation system. There is also a study that extended the Underwood's equation for designing the thermally coupled and dividing wall for reactive distillation [49]. One ground-breaking literature worth discussing is the work of Tedder and Rudd [50] that introduced the usage of ease of separation index (ESI) to distinguish the overall performance of several different ternary distillation configurations, which include the total heat demand and the capital cost. They attributed the energy-saving efficiency of the different thermally coupled distillation columns (TCDS) to several key variables such as the feed composition, the relative volatility, and the purity required in the product streams. Another work worth mentioning here is the investigation carried out by Agrawal and Fidkowski [6] where they compared the thermodynamic efficiencies of five different thermally coupled ternary distillation configurations (Fig. 1) for separation of ideal saturated liquids. In their investigation, they employed the calculation method they previously developed for calculating the thermodynamic efficiency of an ideal binary distillation system [51]. The thermodynamic efficiency calculations reported by Agrawal and Fidkowski [6] covered a wide range of relative volatilities and feed compositions, such as feed with equimolar composition or feed that is rich in one of the components. For each class of composition mixture, the thermodynamic efficiency of the different thermally coupled configuration can be analysed based on their corresponding relative volatilities. One key takeaway from their studies is that the thermodynamic efficiency for the fully thermally-coupled (i.e. Petlyuk) configuration is limited to only certain ranges of feed compositions and relative volatilities, despite having the lowest heat demand for ternary distillation. In comparison to the Petlyuk (i.e. fully thermally coupled) configuration, the thermally-coupled distillation with side-rectifier or side-stripper tends to provide better thermodynamic efficiency. Nevertheless, it is worth to note that the heuristic introduced by Tedder and Rudd and Agrawal and Fidkowski are only valid for separation of ideal saturated liquids [6,52] while no existing study had analysed the energy-saving efficiency in the complex distillations (i.e. extractive distillation, reactive distillation, and etc.), in the same manner as those conducted by Agrawal and Fidkowski for the ideal distillation system [6]. Here, we would like to reiterate that there is also no study that evaluates the applicability of the variables (e.g. feed composition, relative volatility) that determine the energy-saving efficiency in the case of TCDS as revealed by Tedder and Rudd to the intensified extractive distillation case [50]. Therefore, this study aims to fill in the gap of existing studies where it has not yet been established what are the variables that affect the energy-savings and under what conditions the intensified processes (i.e. thermally coupled or dividing-wall) of these complex (i.e. azeotropic) distillation systems present energy-savings.

Here, we try to analyse, in a preliminary way, the energy-saving efficiency of the different intensified extractive distillation processes through three case studies along with the studies that reported similar results in open literature where these energy-intensified processes (e.g. TCED, EDWC, and SSED) do not provide any energy-saving relative to the CED. Our intention here is to provide insights and preliminary conclusions that open a field of study for a more detailed and in-depth analysis, so that future research can be directed towards exploring other possible explanations for these interesting cases on where and when these energy-intensified processes do not provide any energy-savings in comparison to the CED. We also aim to demonstrate that the heuristics developed in the previous studies [6,50] to determine the energy-savings in the TCDS are extendable to the intensified extractive distillation.

The rest of the paper is arranged as follows. Section 2 explains the different case studies presented in this work. The results that are discussed in Sections 3 and Section 4 concludes this work while Section 5 provides several recommendations for future work.

2. Case studies

In Section 1, we presented three existing studies in open literature, which demonstrated that their corresponding energy-intensified processes do not provide any energy-saving relative to their conventional base case. Nonetheless, these studies did not explicitly explain why the corresponding energy-intensified processes could not provide any energy-savings relative to their conventional base case (e.g. CED) for the separation of azeotropic mixture. In this section, we present three additional case studies and attempted to analyse, in a preliminary way, why these energy-intensified processes do not provide any energy-saving relative to the base case (e.g. CED). Note that the energy-intensified processes for all these three case studies, to our knowledge, have not been investigated in any of the open-literature. Here, all the case studies are simulated following their corresponding product specification as outlined in each Section, the simulation of which was conducted using Aspen Plus V11.

Then, it is worth noting that all the case studies in this work are distillation-based processes, which contain various types of decision variables, such as discrete or continuous, which form a mixed integer nonlinear programming (MINLP) problem that can be effectively solved by using stochastic optimisation. Among the different stochastic optimisation available today, the particle swarm optimisation (PSO) has the advantage of exceptionally low computational time and has been applied to optimise the distillation-based processes [5,53,54], represented by Eq. (1):

$$\begin{aligned} &\min_{x\in \mathrm{R}} f(x) = \mathrm{TAC} \\ &\mathrm{R} = \{y\ \&\ z\} \\ &\mathrm{Subjectto}\left\{p_i \geq p_i^{\mathrm{desired}}, i = 1, 2, \cdots,\ \mathrm{n}\right\} \end{aligned} \tag{1}$$

The objective function ($f(x)$) here is to minimise the TAC and the MINLP is bounded by the product purities (p_i^{desired}) based on respective cases. The y and z in Eq. (1) are the discrete and continuous decision variables, respectively, which include the total number of stages in each column, fresh feed and solvent feed tray locations, reflux ratio, distillate rate, side-stream location, side-stream flowrate, and solvent flowrate. The objective function, bounds, and design variables for each case are integrated with the PSO in MATLAB *via* the ActiveX technology and the overall optimisation procedure is graphically illustrated by Fig. 2. The detailed description for the PSO is made available in Appendix A (Supporting Information).

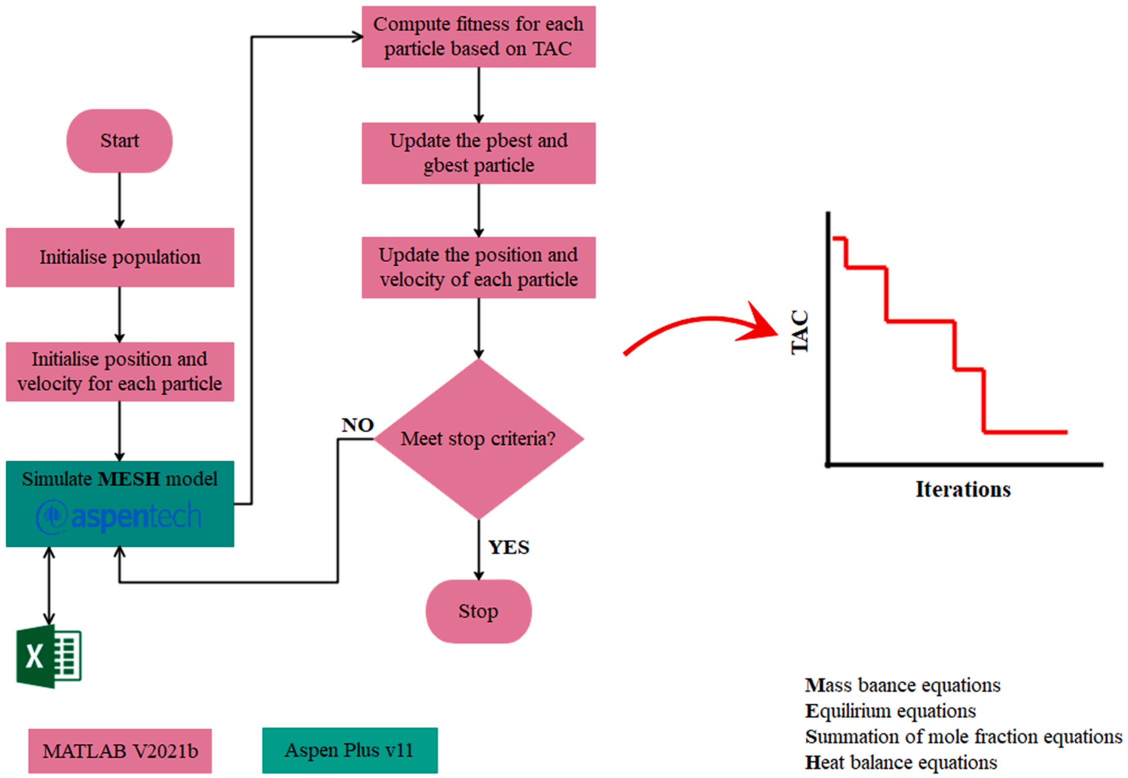

Fig. 2. The PSO optimisation algorithm employed in this work.

2.1. Binary separation of THF and ethanol

The first case study deals with the CED using EG for the binary separation of THF and ethanol from the work of Wang et al. [55] (Fig. 3). THF and ethanol are commonly used as organic solvents in chemical and pharmaceutical industries and thus, the separation and recovery of these individual components have become the subject of interest in these aforementioned industries [56]. However, the mixture of THF and ethanol forms a minimum-boiling azeotrope in the binary system such that the individual component cannot be effectively separated by using ordinary distillation techniques. The CED contains two main columns, i.e. an EDC and an SRC. In the EDC, the fresh feed containing the binary azeotropic mixture and the solvent is fed into the column and the separation takes place where the light product (i.e. THF) is separated and obtained from the distillate while the remaining component containing mainly ethanol and the EG solvent mixture are obtained from the bottom of the EDC and is then directed to the SRC (i.e. second column) for final separation and solvent recovery purpose. In the SRC, the ethanol is obtained from the distillate while the regenerated EG solvent that comes out from the bottom of the SRC is cooled prior to recycling back to the EDC. In most scenario, a solvent make-up flow is used to compensate the solvent that were lost during the distillation processes (i.e. EDC and

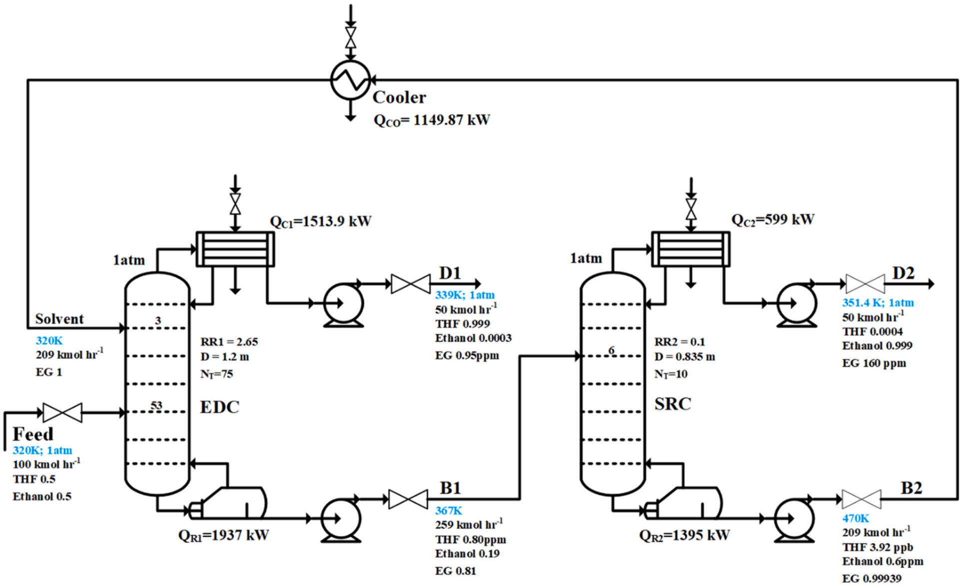

Fig. 3. CED using EG for binary separation of THF and ethanol (Reproduced from previous work [55]).

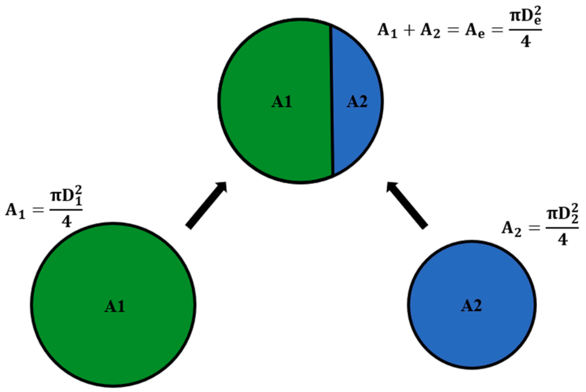

Fig. 4. Illustration for equivalent diameter calculation.

SRC) (not shown in Fig. 3).

To date, our literature survey has indicated that there are no existing studies that have investigated the potential application of the energy-intensified TCED, SSED, and EDWC for reducing the energy consumption of the CED. Following this, we explore the possibility of reducing the energy consumption of the CED by applying these aforementioned energy-intensified technologies. All the three energy-intensified configurations (i.e. TCED, SSED, and EDWC) are optimised using PSO, the bounds, and design variables for each configuration is made available in Appendix B (Supporting Information). For the TAC, it was calculated using similar basis employed by previous work given in Table 1, since the present case study was reproduced based on their work [55].

2.2. *Ternary separation of TBA, ethanol, and water*

The second case study focuses on the ternary separation of TBA, ethanol, and water using EG as a solvent in a DCRED derived from the work of Zhang et al. [58] (Fig. 5). Here, TBA is commonly used as an organic solvent in the pharmaceutical industry, identical to the application of THF in the previous case study. In the hybrid process of DCRED, the water is first removed by reacting it with ethylene oxide (EO) in the reactive-extractive distillation column (REDC) to form EG, which subsequently acts as a solvent (i.e. entrainer) to facilitate the separation between the two remaining components (i.e. TBA and ethanol) in the same column (i.e. REDC). The ethanol leaves from the top of the REDC as the distillate while the mixture of TBA and EG is directed to the SRC for subsequent separation where the TBA leaves as the distillate. The regenerated EG leaves from the bottom of the SRC and is further cooled before it is being recycled back to the REDC. During the recycled process, a portion of the solvent (i.e. EG) is purged out from the system to prevent excessive EG that will be recycled back to the REDC. Such hybrid configuration has become increasingly popular for the separation of ternary azeotropic mixture in the last 2 years [5,26, 58–60]. Here, after reproducing the DCRED from previous work [58] as depicted in Fig. 5, we explore the possibility of reducing the energy consumption through side-stream DCRED (SS-DCRED) and thermally coupled DCRED (TC-DCRED). Both the aforementioned configurations are optimised using PSO, the bounds, and design variables for each configuration is made available in Appendix C (Supporting Information). The DW-DCRED configuration however is not investigated in the present study since it has been investigated in another work [29].

Table 1
Economic basis for TAC calculation (Reproduced from previous work [55]).

Column sizing
Column diameter (D)[1] = Calculated automatically from Aspen Plus
Column Height (H) = 1.2 × 0.61 × (Number of trays (N_T) − 2)
Capital cost = $17{,}640 \times (D)^{1.066} \times (L)^{0.802}$
Condenser and Reboiler sizing (Area in m^2)
Heat transfer coefficient (K_C) = 0.852 kW K^{-1} m^{-2}
Heat transfer coefficient (K_R) = 0.568 kW K^{-1} m^{-2}
Differential temperature (ΔT_C) = reflux-drum temperature – 310 K
Differential temperature (ΔT_R) = steam temperature – base temperature
Area (A_C) = $\frac{Q_C}{K_C \times \Delta T_C}$
Capital cost = $7296\ (A_C)^{0.65}$
Cooler sizing (Area in m^2)
Heat transfer coefficient (K_{CO}) = 0.852 kW K^{-1} m^{-2}
Log mean differential temperature (ΔT_{CO}) = process temperature at inlet and outlet of cooler – 310 K
Area (A_{CO}) = $\frac{Q_{CO}}{K_{CO} \times \Delta T_{CO}}$
Capital cost = $7296\ (A_{CO})^{0.65}$
Energy cost
High pressure steam = $ 9.88 per GJ (527 K)
Medium pressure steam = $ 8.22 per GJ (457 K)
Low pressure steam = $ 7.72 per GJ (433 K)
Cooling water for cooler = $ 0.354 per GJ
Electricity for condenser = $ 16.9 per GJ
TAC
$$\mathrm{TAC} = \frac{\text{Total capital cost}}{\text{payback period}} + \text{annual energy cost}$$
Payback period = 3 years

2.3. *Ternary separation of THF, ethanol, and water*

The third case study is analogous to Case 2, which relies on the hybrid DCRED using EG as a solvent for separating the ternary azeotropic mixture of THF, ethanol, and water. This case is also originated from the work of Zhang et al. [58] (Fig. 6). Since both Cases 2 and 3 use identical processes (i.e. DCRED), the corresponding process flow diagram is no longer elaborated here. Analogous to Case 2, we explore the possibility of reducing the energy consumption through SS-DCRED and TC-DCRED using the reproduced simulation from previous work [58]. In addition, we also simulated the DW-DCRED configuration, which is not covered in Case 2. The SS-DCRED, TC-DCRED, and DW-DCRED configurations are optimised using PSO, the bounds, and design variables for each configuration is made available in Appendix D (Supporting Information).

3. Results and discussion

3.1. *Binary separation of THF and ethanol*

The optimised flowsheet for the TCED, EDWC, and SSED are depicted in Fig. 7, with the optimisation results given in Fig. S1 (Supporting Information). Upon comparing the energy-intensified TCED (Fig. 7(a)), EDWC (Fig. 7(b)), and SSED (Fig. 7(c)) against the CED (Fig. 3), it appears that all the energy-intensified processes do not provide any energy-saving relative to the CED. The reboiler energy for the TCED, EDWC, and SSED increases by 6%, 7%, and 6%, respectively, in comparison to the CED. These findings are in contrast with literature, which reported that these energy-intensified processes (e.g. TCED and EDWC) typically reduce the energy consumption by up to 30% [16–19].

In Fig. 7(a) and 7(b), note that the vapour interconnection stream (IV) between EDC and SRC contains high purity (i.e. amount) of the intermediate product (i.e. ethanol) in both the TCED and EDWC. It appears that these high amount of the intermediate product (i.e. ethanol) that was supposedly discharged through the distillate of the SRC (D2), is being redirected back to the EDC. Since the liquid and vapour internal flowrates of the EDC remain identical to those of CED (a point that will be discussed in next paragraph), it can therefore be deduced that the high amount of intermediate product, which comes from the SRC through the vapour interconnection stream (i.e. IV) is being sent back to the SRC through the liquid interconnection stream (IL). This indicates that there is an accumulation of the intermediate product in the interconnection stream, causing inefficient separation. Such observation was

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[1] The equivalent diameter (D_e) is used for the dividing wall configuration, as illustrated in Fig. 4).

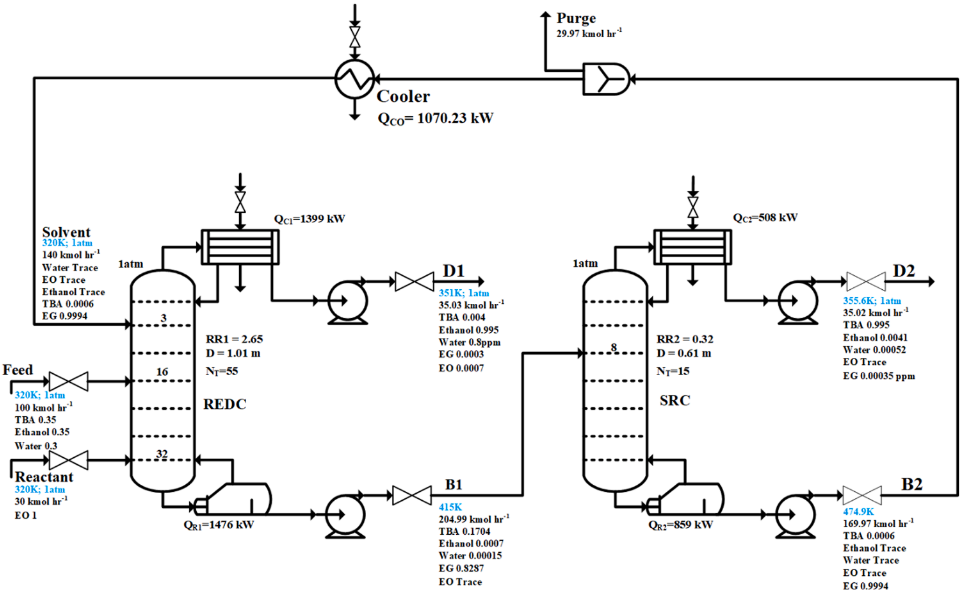

Fig. 5. DCRED using EG as solvent for separation of TBA, ethanol, and water (Reproduced from previous work [58]).

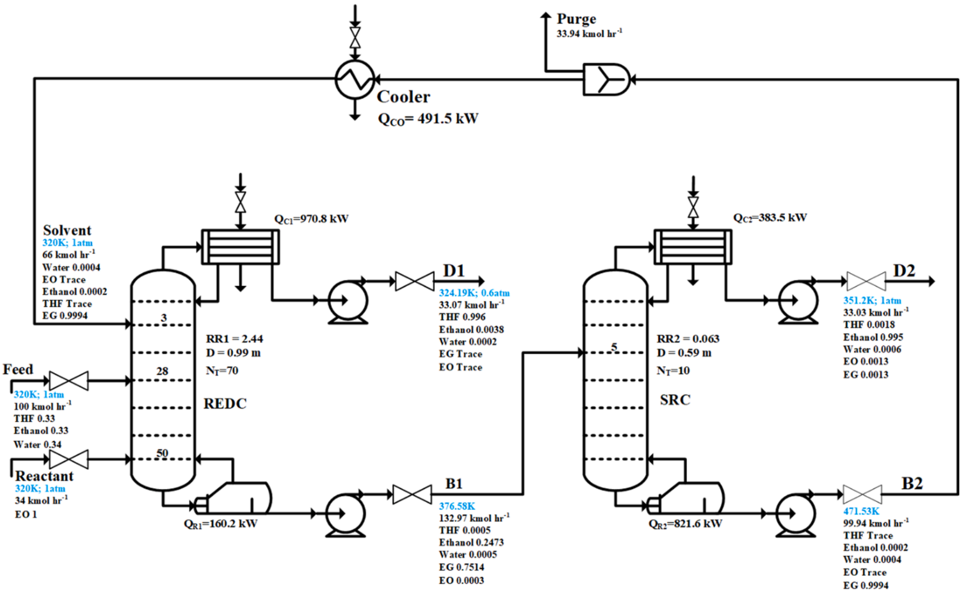

Fig. 6. DCRED using EG as solvent for separation of THF, ethanol, and water (Reproduced from previous work [58]).

supported by the data we analysed from the existing studies reported in Section 1 where the second TCED configuration reported by Zhao et al. [30] that does not save energy, displayed similar characteristic where the interconnection stream contains mainly the intermediate component relative to the first TCED that provides significant energy-savings. Similar trend was observed from the work of Yang et al. [29] where the composition of the intermediate component in the interconnection stream of the DW-DCRED is relatively higher than the DCRED. This possibly explains why the DW-DCRED did not provide any energy-saving relative to the DCRED in previous study [29]. In addition to the similar observations with previous works, such explanation further aligns with the findings of several previous publications for conventional distillation-based processes, which showed that the interconnecting flows have direct effects on the energy consumption and bad values generally translate to a poor energy-savings for the thermally coupled arrangements or it can even be more energy consuming relative to the conventional configurations [18,61–65]. For instance, Amezquita-Ortiz et al. [66] reported that a lower values of interconnection flowrate generally translate to a reduction in energy consumption for the thermally coupled system. The effect of interconnection flowrate on the reboiler duty for the thermally coupled system is also reported in Ref. [66]. Altogether, it appears that the composition and flowrate of the interconnecting stream also play an important role on the energy consumption and such observation can be indirectly linked to the heuristic reported by Tedder and Rudd [50] where they associated the energy-savings to several variables such as the feed composition, relative volatility, and the purity required in the product streams. However, the previously developed heuristic is only valid for non-azeotropic mixtures, ternary mixtures, and TCDS while the present study focuses on the separation of azeotropic mixture [50]. Therefore, we are unable to analyse our case further using the previously developed heuristic (i.e. ESI) [50] and more validation must be made to ensure that the heuristic can be extended to the separation of azeotropic mixture. As indicated in Section 1, we would like to reiterate that our literature survey has

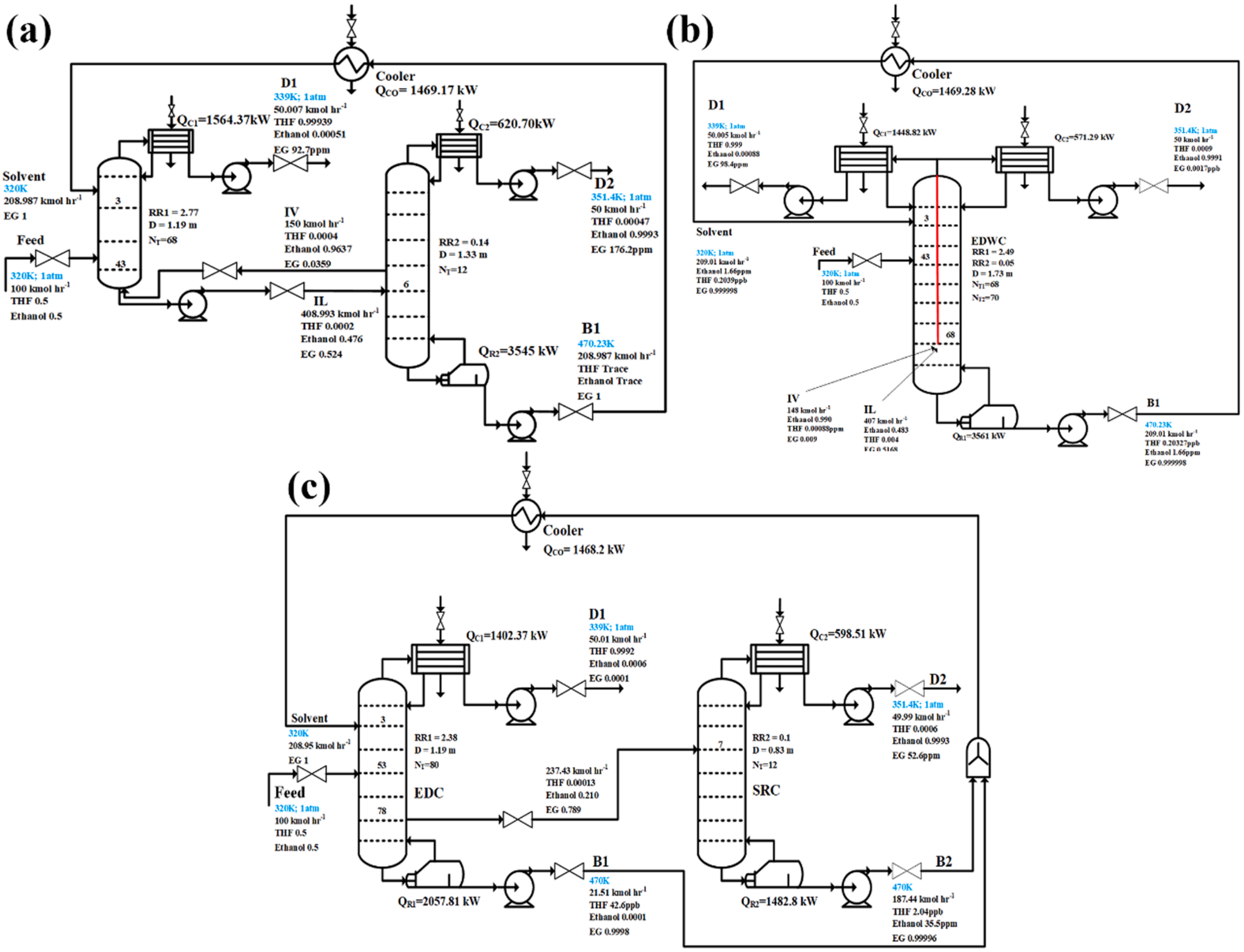

Fig. 7. Different energy-intensified processes for the binary separation of THF and ethanol; optimised (a) TCED, (b) EDWC, and (c) SSED.

indicated that the heuristic identical to those previously developed for ideal distillation system [50] has never been reported explicitly in literature for the case of azeotropic mixture. Following this, future research must be directed towards developing a methodology similar to those developed by Tedder and Rudd [50], for formulating similar heuristic for other types of distillation-based techniques (e.g. reactive distillation and extractive distillation).

Table 2
Internal flowrate comparison for the different energy-intensified processes for separation of THF and ethanol.

Column	Average flowrate based on	CED	TCED	EDWC	SSED
EDC	Whole column	195	199.3	186.1	177.2
SRC	Whole column	57	n/a	n/a	55.65
	Above side-draw location	n/a	56.28	52.4	n/a
	Below side-draw location	n/a	230.2	207.77	n/a
Total reboiler duty (kW)		3332	3545	3561	3540

Then, another possible causes for such increase in the energy consumption, in our opinion, can be attributed to the increase in the vapour flowrate in the column. According to Finn [67], the increase in column internal vapour flowrate generally translate to a higher energy consumption since the energy consumed by a distillation column is directly related to the column internal vapour flowrate. Likewise, it generally requires a larger column diameter and thus, increases the column capital cost [47]. Therefore, vapour flowrate is a very good indicator for evaluating different distillation systems since it can usually be determined quite easily. Table 2 shows the column internal vapour flowrate for different energy-intensified processes relative to the CED. Here, the internal vapour flowrate of the EDC for all cases are calculated based on the average column internal flowrate. Similarly, the internal vapour flowrate of the SRC for the CED and SSED also employed the average column internal flowrate. The SRC for the TCED and EDWC, on the other hand, has two vapour internal flowrates. The first one is the average flowrate of all stages above the side-draw location while the second is vice-versa (i.e. the average flowrate of all stages below the side-draw location). One interesting observation worth noting is that in general, the average internal vapour flowrate below the side-draw location should satisfy two criterias. The first criteria is that the value must be higher than the average flowrate above the side-draw location because most of the vapour is directed back to the EDC through the side-draw. In addition, the value must also be higher than the average internal vapour flowrate in the EDC column because all the vapour flowrate in the EDC comes from the SRC. For the case of TCED and EDWC, the internal vapour flowrate below the side-draw location is used as subsequent comparison. Altogether. it was revealed that almost all the energy-intensified processes have higher total vapour internal flowrate in comparison to the CED. Such finding is also in agreement with the explaination of previous study in a recent investigation on the unfavorable energy integration of reactive dividing wall column [68]. Here, we believe that the increase in vapour internal flowrate below the side-draw location in the SRC, in particular, plays an important role in the present case relative to the EDC, especially for the case of TCED and EDWC, as these energy-intensified processes were simulated through eliminating the reboiler unit of the EDC instead of SRC. This is supported by one of the data obtained from previous work [29] on the DW-DCRED and DCRED for the ternary azeotropic separation of TBA, ethanol, and water. Here, note that the difference between the dividing wall in our case study and previous work is that the dividing wall configuration from previous study was simulated through eliminating the reboiler unit of the SRC instead of the REDC and therefore, the increase in vapour flowrate in the REDC increases the energy consumption for previous study. In essence, our simulation suggested that the increase in the vapour internal flowrate in the column where the reboiler unit is present, generally increases the energy consumption of the system. Such observation is consistent with previous study where Amezquita-Ortiz et al. [66] observed that in the double column thermally coupled system, the column diameter for one column (e.g. C1) is smaller than the referred base case while the diameter of the other column (e.g. C2) is relatively larger, having a greater number of stages and a larger diameter. They observed that the diameter has a negative effect on the distribution of the internal flows, which increases the re-flow ratio, subsequently generating large interconnection flows. In the present case, the size (i.e. diameter and number of stages) of the first column for the TCED (Fig. 7(a)) and EDWC (Fig. 7(b)) is relatively smaller than the base case (Fig. 3) while the size (i.e. diameter and number of stages) of the second column is vice versa. In our opinion, this increases the internal flowrate in the intensified system, which aligned with the observation made by previous study [61].

In terms of TAC, all the energy-intensified configurations do not provide any reduction in comparison to the CED (Table 3). The TAC for the TCED, EDWC, and SSED increased by 15%, 19%, and 17%, respectively, relative to the CED. Such increase was attributed to the marginal increase in the reboiler energy and steam cost. Other than that, the capital cost for all energy-intensified processes also increases by marginal, mainly due to the higher vapour and liquid exchanging stream in between both columns, which is in agreement with previous studies [30, 57]. There is a also tremendous increase in the operation cost for the SSED relative to the CED and this was mainly due to the reboiler temperature of the EDC in the SSED is higher than the CED at 470 K, and thus, requiring high-pressure steam to be used for supplying the required heat-duty to the EDC, instead of the low-pressure steam as in the case of CED.

Overall, it was demonstrated that all the energy-intensified processes investigated in this case does not provide any energy-savings relative to the CED.

3.2. *Ternary separation of TBA, ethanol, and water*

The optimised flowsheet for the SS-DCRED and TC-DCRED are given in Fig. 8, with the optimisation results given in Fig. S2 (Supporting Information). Analogous to Case 1, the energy-intensified processes investigated here, i.e. SS-DCRED and TC-DCRED, do not provide any reduction in energy consumption relative to the conventional DCRED. The reboiler energy for the optimised SS-DCRED and TC-DCRED increases by 24% and 55%, with respect to the conventional DCRED. These findings nevertheless are in agreement with previous study, which addresses the same separation mixture using DW-DCRED and showed that it does not contribute towards any energy-saving [29].

Table 3
Result summary between CED against the optimised TCED, SSED, and EDWC.

Parameters	CED	TCED	EDWC	SSED
Total reboiler duty (kW)	3332	3545	3561	3540
Column cost (10^6 $)	0.55	0.59	0.73	0.61
Exchanger cost (10^6 $)	0.32	0.29	0.28	0.32
Operating cost (10^6 $)	0.85	1.03	1.03	1.03
TAC ($ 10^6 yr^{-1})	1.15	1.32	1.37	1.34

Identical to Case 1, we attributed the increase in energy consumption to the high column internal vapour flowrate in the SRC (Table 4), especially for the TC-DCRED that was simulated by eliminating the reboiler unit of the REDC instead of the SRC. Such justification, again, is consistent with the data we obtained and analysed from previous study [29]. Analogous to Case 1, the vapour interconnection stream (i.e. IV) from the SRC to the EDC in the present case also contains high purity (i.e. amount) of the intermediate product (i.e. TBA), which was supposedly emitted through the distillate of the SRC. In our opinion, this has resulted in the accumulation of the intermediate product in the interconnection stream, causing inefficient separation and such observation aligned with Case 1 and also the data we analysed from the existing studies [30]. Also, we ingeminate that such justification is analogous to the findings from several existing publications for conventional distillation-based processes, which show that bad values of interconnecting flows have direct effects on the energy consumption, thus leading to poor energy-savings for the intensified configurations [18, 61–65]. This observation is also consistent with the observation made by Amezquita-Ortiz et al. [66] where a lower values of interconnection flowrate generally provides a lower energy consumption for the intensified system.

Other than analysing the energy-saving efficiency based on the internal vapour flowrate, we also attempted to analyse it using the methodology employed by Agrawal and Fidkowski [6], where they analysed the energy-saving efficiency of the conventional distillation for ideal mixture based on the relative volatility and feed composition. Here, it is worth noting that we are unable to analyse the energy-saving efficiency for Case 1 because the previously developed methodology was originally expressed for ternary mixture only [6]. For the present Case 2, the feed composition contains equimolar amount of TBA and ethanol (i.e. 35 mol. % each) while the water content is 30 mol. %. The α_{AB} is 3.21. For such mixture, it appears that the most efficient configuration is the modified thermally coupled with direct split (Fig. 1(d)), regardless of whether we assume that such feed mixture belongs to the feed rich in A component (THF), B component (ethanol), or all the three components have equimolar composition, as categorised by previous work [6]. For the feed that is rich in A component, the thermally coupled with side-stripper configuration (Fig. 1(b)) was also reported to be an alternative thermodynamic efficient configuration. In this study, the TC-DCRED was simulated using the side-rectifier configuration and therefore, it appears to have lower thermodynamic efficiency and does not provide any energy-saving if we assume that the previously developed heuristic is valid for the separation of azeotropic mixture [6]. However, further investigation must be made to validate the applicability of the previously developed heuristic for separation of azeotropic mixture [6]. It is also interesting to simulate the TCED and EDWC using the modified thermally coupled with direct split or the thermally coupled with side-stripper to investigate its energy-saving potential for Case 2.

For the TAC, both the optimised TC-DCRED and SS-DCRED do not provide significant reduction relative to the DCRED (Table 5), identical to Case 1. The TAC for the TC-DCRED and SS-DCRED increased by 62% and 31%, respectively, relative to the DCRED. Such increase was attributed to the large increase in both the steam cost and reboiler energy, which further translates to a remarkable increase in the exchanger cost. Altogether, it was demonstrated that the energy-intensified TC-DCRED and SS-DCRED do not provide any energy-saving for the separation of TBA, ethanol, and water, analogous to the findings reported by previous study for the DW-DCRED [29].

3.3. *Ternary separation of THF, ethanol, and water*

The resulting flowsheet for the optimised TC-DCRED, DW-DCRED, and SS-DCRED are given in Fig. 9. Analogous to Cases 1 and 2, all the

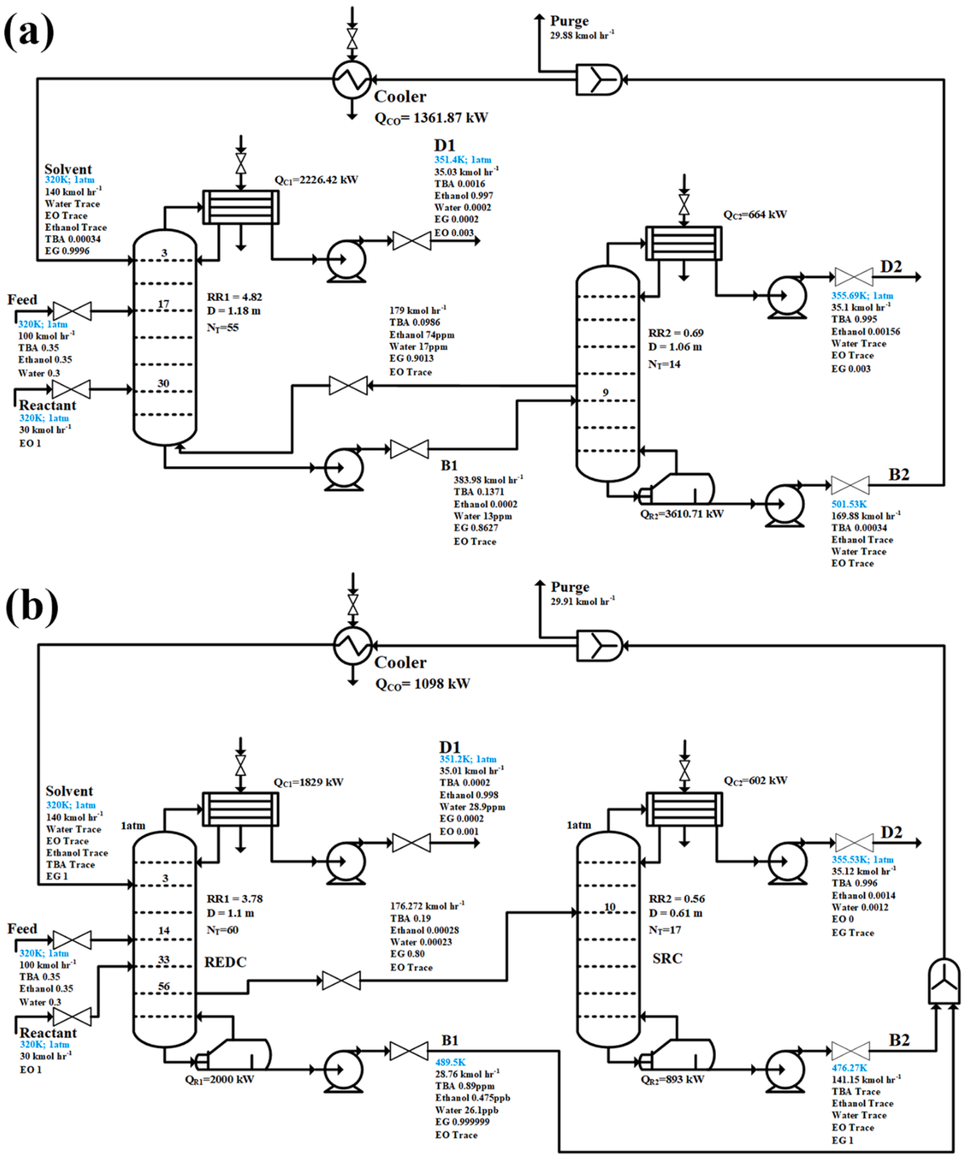

Fig. 8. Different energy-intensified processes for separation of TBA, ethanol, and water; optimised (a) TC-DCRED and (b) SS-DCRED.

Table 4
Internal flowrate comparison for the SS-DCRED, TC-DCRED, and DCRED for separation of TBA, ethanol, and water.

Column	Average flowrate based on	DCRED	TC-DCRED	SS-DCRED
REDC	Whole column	142	218.1	178
SRC	Whole column	36.7	n/a	50
	Above side-draw location	n/a	48.62	n/a
	Below side-draw location	n/a	219.72	n/a
Total reboiler duty (kW)		2335	3610	2893

Table 5
Result summary between DCRED against optimised TC-DCRED, and SS-DCRED.

Parameters	DCRED (Literature)	TC-DCRED	SS-DCRED
Total reboiler duty (kW)	2335	3610	2893
Column cost (10^6 $)	0.40	0.50	0.46
Exchanger cost (10^6 $)	0.29	0.51	0.34
Operating cost (10^6 $)	0.61	1.05	0.84
TAC ($ 10^6 yr^{-1})	0.86	1.39	1.13

energy-intensified processes investigated here, i.e. TC-DCRED, DW-REDWC, and SS-DCRED do not provide any reduction in energy consumption relative to the conventional DCRED. The reboiler energy for the TC-DCRED, DW-REDWC, and SS-DCRED increases by 24%, 15%, and 15%, with respect to the conventional DCRED. These results trend again are in agreement with previous study for the DCRED system, which demonstrated that the intensified configurations for the DCRED system does not contribute towards any energy-saving [29], despite previous study was for a different mixture.

Identical to Cases 1 and 2, one possible explanation for the increase in energy consumption was attributed to the high column internal vapour flowrate (Table 6). Contrary to Cases 1 and 2 where the intensified configurations were simulated by eliminating the reboiler unit of REDC/EDC instead of the SRC, the intensified configurations (i.e. TC-DCRED and DW-DCRED) in the present case were simulated by eliminating the reboiler unit of the SRC for the sake of easier convergence. Therefore, the internal vapour flowrate of the SRC in this case are calculated based on the average column internal flowrate. On the other hand, the internal vapour flowrate of the EDC for the TC-DCRED and DW-DCRED has two values, i.e. the first one for all the stages above the side-draw location while the second is for all the stages below the side-

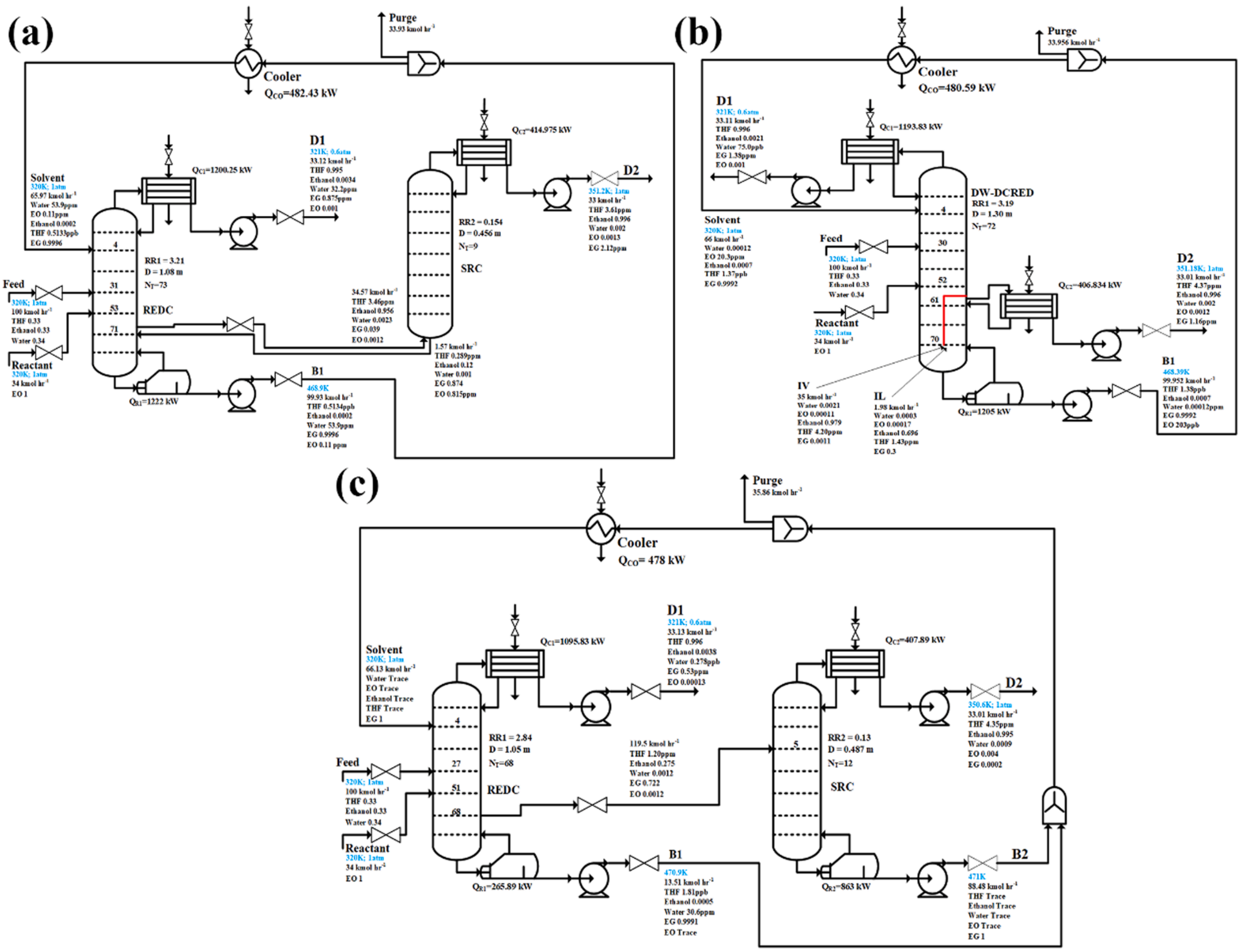

Fig. 9. Different energy-intensified processes for the ternary separation of THF, ethanol, and water; optimised (a) TC-DCRED, (b) DW-DCRED, and (c) SS-DCRED.

Table 6
Reboiler duty and internal flowrate comparison between DCRED against the optimised TC-DCRED, DW-DCRED, and SS-DCRED for separation of THF, ethanol, and water.

Column	Average flowrate based on	DCRED	TC-DCRED	DW-DCRED	SS-DCRED
REDC	Whole column	95	n/a	n/a	87
	Above side-draw location	n/a	95.3	96.6	n/a
	Below side-draw location	n/a	60.3	57.4	n/a
SRC	Whole column	33	38.97	38.75	37.5
Total reboiler duty (kW)	981.8	1,222	1,125	1,129	

draw location. In this case, the average internal vapour flowrate above the side-draw location is generally higher than the average flowrate below the side-draw location because most of the vapour in the REDC is directed to the SRC through the side-draw (Table 6). As for the SRC, the average internal vapour flow is generally lower than the REDC because all the vapour flowrate in the SRC comes from the REDC. For subsequent comparison, the internal vapour flowrate above the side-draw location is used for the case of TC-DCRED and DW-DCRED. From Table 6, it was demonstrated that the TC-DCRED and DW-DCRED have higher total vapour internal flowrate in comparison to the DCRED. Such finding aligned with our results obtained from Cases 1 and 2 and is also in agrement with previous studies [68]. It is also consistent with the fact that a lower value of interconnection flowrate facilitates reduction in energy consumption for the energy-intensified configurations [66]. Here, note that the size (i.e. diameter and number of stages) of the second column for the intensified system (Fig. 9(a) and 9(b)) is relatively smaller than the base case (Fig. 6) while the size (i.e. diameter and number of stages) of the first column is vice versa, because the intensified configurations in the present case were simulated by eliminating the reboiler unit of REDC/EDC (first column) instead of the SRC (second column), as indicated in earlier section. In our opinion, this increases the internal flowrate of the intensified system, which is consistent with the observation made by previous study [66] because the diameter has a negative effect on the distribution of the internal flows, which increases the re-flow ratio, subsequently generating large interconnection flows. For the case of SS-DCRED, it was observed from Table 6 that the column internal vapour flowrate is similar to the DCRED, with the conventional DCRED having a slightly higher extent by about 9% (Table 6). Note that the SS-DCRED is different from DW-DCRED and TC-DCRED, and therefore, our previous justification on the increase in vapour flowrate for DW-DCRED and TC-DCRED that generally signifies an increase in the energy consumption does not apply. Therefore, future research must be diverted towards exploring these interesting cases.

Identical to Case 2, we also attempted to analyse the energy-saving efficiency using the heuristic developed by Agrawal and Fidkowski [6], based on the relative volatility and feed composition. For the present Case 3, the feed composition contains equimolar amount of THF and ethanol (i.e. 33 mol. % each) while the remainder is water of 34 mol. %. The α_{AB} is 0.86. For such mixture, the most efficient configuration is the modified thermally coupled with direct split (Fig. 1(d)), identical to the explanation we provided in Case 2. As indicated earlier, the TC-DCRED and DW-DCRED here were simulated using the side-rectifier configuration and therefore, it is expected for the thermodynamic efficiency to be lower, which does not facilitate any energy-saving if we assume that the previously developed heuristic by Agrawal and Fidkowski [6] is valid for the separation of azeotropic mixture. Another alternative energy-efficient configuration is the thermally coupled with side-stripper (Fig. 1(b)) if we assume that the feed is rich in A component (THF). Here, future research can explore the possibility of reducing the energy consumption for Case 3 by simulating the modified thermally coupled configuration with direct split or the thermally coupled with side-stripper configuration. Nonetheless, we reiterate that further investigation must be conducted to validate the applicability of the previously developed heuristic for separation of azeotropic mixture [6].

Table 7 shows the TAC comparison between the optimised TC-DCRED, DW-DCRED, and SS-DCRED against the DCRED for the separation of THF, ethanol, and water. From Table 7, it becomes clear that the optimised TC-DCRED, DW-DCRED, and SS-DCRED provides a higher TAC by about 23%, 13%, and 7% relative to the DCRED. Such increase was mainly associated to the increase in the reboiler energy and steam cost. Moreover, the capital cost for all energy-intensified processes also increases by marginal. Altogether, it was demonstrated that all the energy-intensified DCRED does not provide any energy-saving and reduction in TAC relative to the DCRED for the separation of THF, ethanol, and water.

Table 7
Result summary between DCRED against the optimised TC-DCRED, DW-DCRED, and SS-DCRED.

Parameters	DCRED (Literature)	TC-DCRED	DW-DCRED	SS-DCRED
Total reboiler duty (kW)	981.8	1,222	1,125	1,129
Column cost (10^6 $)	0.45	0.48	0.55	0.46
Exchanger cost (10^6 $)	0.24	0.28	0.27	0.28
Operating cost (10^6 $)	0.28	0.36	0.33	0.32
TAC ($ 10^6 yr^{-1})	0.54	0.61	0.61	0.58

4. Conclusion

In conclusion, we presented three case studies where their corresponding energy-intensified processes (e.g. TCED, EDWC, and SSED) do not provide any energy-saving relative to the CED. In light of the results obtained in this study and upon association with similar cases reported in open literature, our preliminary analysis suggested that for separation of azeotropic mixture, the composition and flowrate of the interconnecting stream in the TCED and EDWC plays an important role on the energy consumption. In particular, the high composition of the intermediate component in the liquid/vapour interconnection stream generally translate to poor energy saving in the case of energy-intensified configurations. This was supported by the similar data trend we observed from several existing studies where their corresponding energy-intensified configurations do not provide any energy-saving relative to the conventional base case [16,17]. In essence, bad values of the interconnecting flow and composition generally translate to a poor energy-savings and this is analogous to the results reported by several existing studies for conventional distillation-based processes [18,61–65].

In addition, the results from our case studies also suggested that the increase in the high column internal vapour flowrate translates to a higher heat energy consumption required by the distillation column, which align with the results reported by a recent study [68]. This is especially the case where the reboiler unit is present and increasing the vapour flowrate generally increases the energy consumption of that particular column. Such observation was supported by the data we obtained and analysed from previous work [29].

Lastly, we also attempted to analyse, in a preliminary way, the case studies presented in this work using the previously developed heuristic for separation of ideal mixture [6,50] and it was revealed that these developed heuristic can potentially be extended to evaluate the energy-efficiency for separation of azeotropic mixture.

Altogether, it is hoped that these three interesting case studies served as an introduction to create the attention and raise the awareness of future researchers to start exploring under when and where these energy-intensified processes do not provide any energy-savings in comparison to the CED, for the separation of azeotropic mixture.

5. Recommendation for future work

Several areas for future work stemming from both the simulation results and the analyses we carried out on existing publications that reported identical results are as follows:

1 **In depth analysis on the effect of interconnection stream flowrate**: An in-depth analysis should be carried out to analyse how different flowrates will affect the composition of the intermediate component and subsequently, determine how the composition of the intermediate component will affect the energy-savings in the intensified configurations. Such analysis can additionally be link with the the heuristic reported by Tedder and Rudd [50] for ideal distillation, where they associated the energy-savings to several variables such as the feed composition, relative volatility, and the purity required in the product streams.

2 **Verifying the validity of the previously developed heuristic for ideal distillation, for complex distillation:** Although in the present study, we attempted to analyse, in a preliminary way, the case studies presented using the previously developed heuristic for separation of ideal mixture [6,50], it should be noted that the previously developed heuristic is only valid for non-azeotropic mixtures, ternary mixtures, and TCDS and therefore, more validation must be made to ensure that the heuristic can be extended to the separation of azeotropic mixture. It is worth reiterating that the heuristic identical to those previously developed for ideal distillation system [50] has never been reported explicitly in literature for the case of azeotropic mixture.

3 **Framework development for energy analysis on complex distillation:** It is also recommended to develop a set of comprehensive methodology, identical to those developed for conventional distillation process, for evaluating the energy-saving efficiency for other types of distillation-based processes (e.g. reactive distillation and extractive distillation).

Data availability statement

All data generated or analysed during this study are available from the corresponding authors on reasonable request.

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.

Data Availability

Data will be made available on request.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.cep.2022.109131.

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