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Improving plant-level heat pump performance through process modifications

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HIGHLIGHTS

- Process change analysis identifies changes that improve a heat pump's performance.
- The split exergy grand composite curve shows the work requirements of a heat pump.
- Proper heat extraction appropriate HP placement and utilization of work potential.

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ABSTRACT

Heat pumps are a promising option to decarbonize the industrial sector. However, their performance at a plant-level can be affected by other process changes. In this work, process changes that improve the heat pump's performance have been identified using Process Change Analysis (PCA), where the background pinch point is used as a reference point for appropriate placement. The effects of the process changes on the heat pump's work requirements are studies by introducing exergy to PCA to form the split exergy grand composite curve. This graph shows the work potential of the streams connected to the heat pump and therefore its work targets. The framework is demonstrated in two case studies. In a biodiesel production plant, it allowed to identify technologies that enhance heat pump performance while reducing overall heating requirements. Here, a heat pump transfers 1.9 MW with a COP of 4.2 but incurs a 40 kW penalty for transferring heat above the background process's pinch temperature. Replacing the wet water washer with a membrane separation unit avoided this penalty, while drastically reducing energy requirements from 0.9 MW to 0.3 MW. in a vinyl chloride monomer-purification process, PCA showed how the extraction of heat by the heat pump impacted the formation of the background pinch, from which an implementation strategy was derived that increased the heat pump's plant-level performance by 6.5% with respect to standard implementation.

1. Introduction

Numerous technologies have been developed to increase performance and reduce CO_2 emissions in the industrial sector. While many options are still in the early stages of development, high-temperature heat pumps are ready to be implemented at an industrial scale [1]. Their estimated energy reduction potential in the European chemical, paper, food and refinery industries is estimated at about 1100 PJ/a [2]. Heat pumps are therefore likely to play a significant role in future energy systems. However, their adoption has been held up by the complexity of finding economically feasible heat pump options and selecting the “right” heat pump technology [3]. This process is further complicated by the heat pumps sensitivity to the deployment of new technologies needed to meet CO_2 reduction targets [4].

A heat pump reduces net heating and cooling requirements by transferring heat from a region with a surplus of heat to a region with a net heat demand [5,6]. These regions can be identified with the help of pinch analysis [7]. More specifically, pinch analysis identifies the

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location in the process, I.e., the pinch point, where further heat transfer from hot to cold streams is limited by a minimal temperature driving force [8]. The region above this point requires a net amount of heat, whereas the region below has a surplus of heat. A heat pump transfers this surplus of heat to the region with a net heat requirement. If a heat pump only partially transfers the heat across the pinch point, as it partially extracts heat from the region with a net heat requirement or supplies heat to the region with a surplus, the heat pump is inappropriately placed. This creates a difference in the amount of heat supplied by the heat pump and the reduction of plant-level heating requirements, known as the inappropriate placement penalty [5,6].

The thermodynamic performance of a heat pump is typically expressed in terms of the “Coefficient of Performance (COP)”, which is the ratio between the amount of heat delivered and the required work. In case a heat pump is inappropriately place and the amount of heat delivered by the heat pump is not the same as the reduction of heating requirements on a plant-level, the plant-level COP is lower than that of the heat pump itself at a unit-level. The work required by the heat pump is needed to transfer the heat from below to above the pinch point. This amount of work is proportional to the exergy difference between the streams connected to the heat pump [9]. This difference is a function of the amount of heat transferred and their temperature difference. Hence, heat pump connections should be taken as close to the pinch point as possible to minimize work requirements [10]. The heat pump's COP is therefore largely determined by the temperature difference between the selected process connections [10]. Process changes near or to the processes that form the pinch point, or even the implementation of the heat pump itself, may change the pinch temperature and the shape of the pinch [11]. These changes can affect the heat pump's COP on a plant-level, as part of the transferred heat may no-longer be across the pinch point. Hence, considering how such changes impact the heat pump's performance is essential in the design process.

The strive for increasing efficiencies has, in most processes, led to a wide variety of plausible newly developed technologies. When looking at a typical chemical process plant, many technologies, or process changes, have been suggested. In the case of a biodiesel production plant, most of these changes have been proposed for either the reaction or the separation section, where changes to catalysts are commonly explored. A review by Bohlouli and Mahdavian [12] listed ten categories, like enzyme base catalyst and heterogeneous alkali metal oxides. Moreso, an overview by Kiss et al. [13], listed seven subcategories of process intensification measures in the reaction section, like membrane reactors and reactive distillation. Both types of process changes may impact the temperature of the pinch point [4]. The time required to assess the sheer number of possibilities and possible interactions often overstretches the time available to process engineers.

The impact of process changes on the plant's pinch point is commonly studied with the help of Process Change Analysis (PCA) [7]. Linnhoff and Vredeveld [14] developed this framework as a combination of the split grand composite curve (Split-GCC), and the plus-minus principle. This framework can be used to explore how a unit relates to the rest of the plant from a heat integration perspective. PCA shows the effect a unit has on the formation of the pinch point by splitting (extracting) processes from the rest of the plant in a (split) grand composite curve. The processes that are not extracted are collectively called the background process. PCA makes explicit whether an extracted process is appropriately placed withrespect to the pinch point of the background process and how it contributes to heat integration characteristics, like self-integrating heat pockets. Dhole and Linnhoff [15] used this framework to explore how current pump-arounds in an existing distillation column could be used to increase heat integration with the background process. Glavic et al., [16,17] showed how PCA could be combined with the appropriate placement rules for energy conversion technologies on the appropriate integration of endothermic and exothermic reactors with PCA. Wiertzema et al. [18] showed how PCA could be used to explore the impact of deploying a new processing unit with a fundamentally different heat profile. In their study, PCA uncovered that the loss of waste heat by electrifying processes in an oxo-synthesis plant increased overall energy requirements, offsetting the envisioned CO_2 savings. These examples all used PCA to assess the impact of already selected technologies on the process's heat integration, whereas the selection of CO_2-mitigating technologies is one of the main challenges faced by engineers. However, PCA also could be a valuable tool in this technology selection process, as it can highlight required changes that improve overall heat integration, and could thus provide a sound basis for assessing decarbonization pathways.

The main premise of this article is that heat pumps are planned to be deployed as a first step to decarbonize the industrial process, and will be accompanied by other process changes to meet CO_2 reduction goals. Here, the goal is to identify process changes that improve the heat pump's plant level performance by reducing appropriate placement penalties. In this study, the concept of exergy will be added to the framework of PCA to directly assess the effects of adding decarbonization technologies next to the heat pump. The overall aim of this article is to show how PCA can help identifying process changes that reduce overall heating requirements whilst increasing the performance of a heat pump and how the placement of the heat pump itself may impact the heat pump's performance. This knowledge will help to identify promising combinations of heat pumps and other mitigation technologies that can increase the combined CO_2 reduction and discard unfruitful options in the early stages of the technology selection process.

2. Method

The overall method of selecting and assessing the impact of sequential process changes on a heat pump's performance consists of three phases: (1) selection of heat pump connections, (2) selection of process changes, and (3) assessment of the impact of process changes on the heat pump's COP.

2.1. Selection of heat pump connections

The basis of the analysis was a consistent process model based on operational process data and chemical equilibria covering over 90% of a real production plants' energy consumption. Impurities were not considered in the model. The specific heat of the considered streams was linearized to allow for a max error of 10% and the temperatures represent the yearly averages. The resulting energy and mass balance were used as input for a pinch analysis, and the results were visualized in a grand composite curve. For the pinch analysis, a minimal temperature difference of 10 °C was adopted. Heat pump connections were defined as the streams closest to the pinch point with a size of at least 10% of the total heating requirements. If multiple streams met this criterion, the ones with the largest heat capacity flowrates were selected. For both, the heat source and the sink, a single process connection is considered to limit the integration cost of the heat pump. This limits the thermal duty of the heat pump's heat sink (Q_{sink}). The required amount of energy needed from the heat source (Q_{source}) was based on Eq. (1):

$$Q_{source} = Q_{sink} - W_{comp}, \tag{1}$$

where, W_{comp} was defined as the work added by the heat pump's compressor, which was approximated based on the exergy values of the heat source (X_{source}) and sink (X_{sink}) and an exergetic efficiency (η_{ex}), as indicated in Eq. (2):

$$W_{comp} = \frac{1}{\eta_{ex}}(X_{sink} - X_{source}), \tag{2}$$

where the exergy values were defined as in Eq. (3):

$$X_i = \eta_c Q_i, \tag{3}$$

Where, $_i$ was either the source or the sink and η_c was the Carnot factor

(1-T_0/T) with the environmental temperature (T_0) set at 15 °C [19]. An exergetic efficiency (η_{ex}) of 0.59 was assumed to compensate for irreversibilities common in a mechanical vapor compression heat pump [20,21]. The planned integration of the theoretical heat pump was done as shown in Fig. 1.a. Three heat extraction options were considered when there was a significant excess of heat available (>10% heat source), as in Fig. 1.a. The first option involved utilizing the heat from the top-end (Q_{top} Fig. 1.b.) of the stream to minimize the temperature lift and compressor work. The remaining thermal duty of the stream was added to the background processes, as depicted in Fig. 1. b. The second option utilized the bottom-end of the stream (Q_{bottom} in Fig. 1.c.) to establish a pinch point and ensure appropriate integration, while the heat from the top-end of the heat source was added to the background process. The third option involved a split integration, extracting heat from the entire temperature range of the source but only from a smaller (split) stream, while the rest of the stream was added to the background process, as in Fig. 1.d. The amount of heat that was extracted from the heat source was determined by solving the energy balance of Eq. (1), where the work added by the compressor was defined by Eq. (2) and Eq. (3). Herein, the outlet temperature of the heat source was iteratively calculated based on the heat capacity flow rate of the stream and the amount of heat required to balance Eq. (1).

The process-heat pump connections were used in a pinch analysis, just as the remaining background processes. Both were visualized in a Split-GCC and a split exergy grand composite curve (Split-EGCC). The latter curve was formed with the introduction of the Carnot factor on the ordinate of the Split-GCC. The Split-EGCC visualises the impact of design choices, like the heat extraction strategy, on the work targets of the heat pumps as these can graphically be deduced with the help of Eq. (3), as in Fig. 1.e.

2.2. Selection of process changes

The process changes, i.e., deployment of decarbonization technologies in the reactor and separation sections, were selected for their ability to reduce overall heating requirements while improving the heat pump's performance by minimizing penalties from inappropriate placement regarding the background process pinch point, i.e., not solely transferring heat across the pinch point of the background process. Only process changes to the background process were explored in this paper,

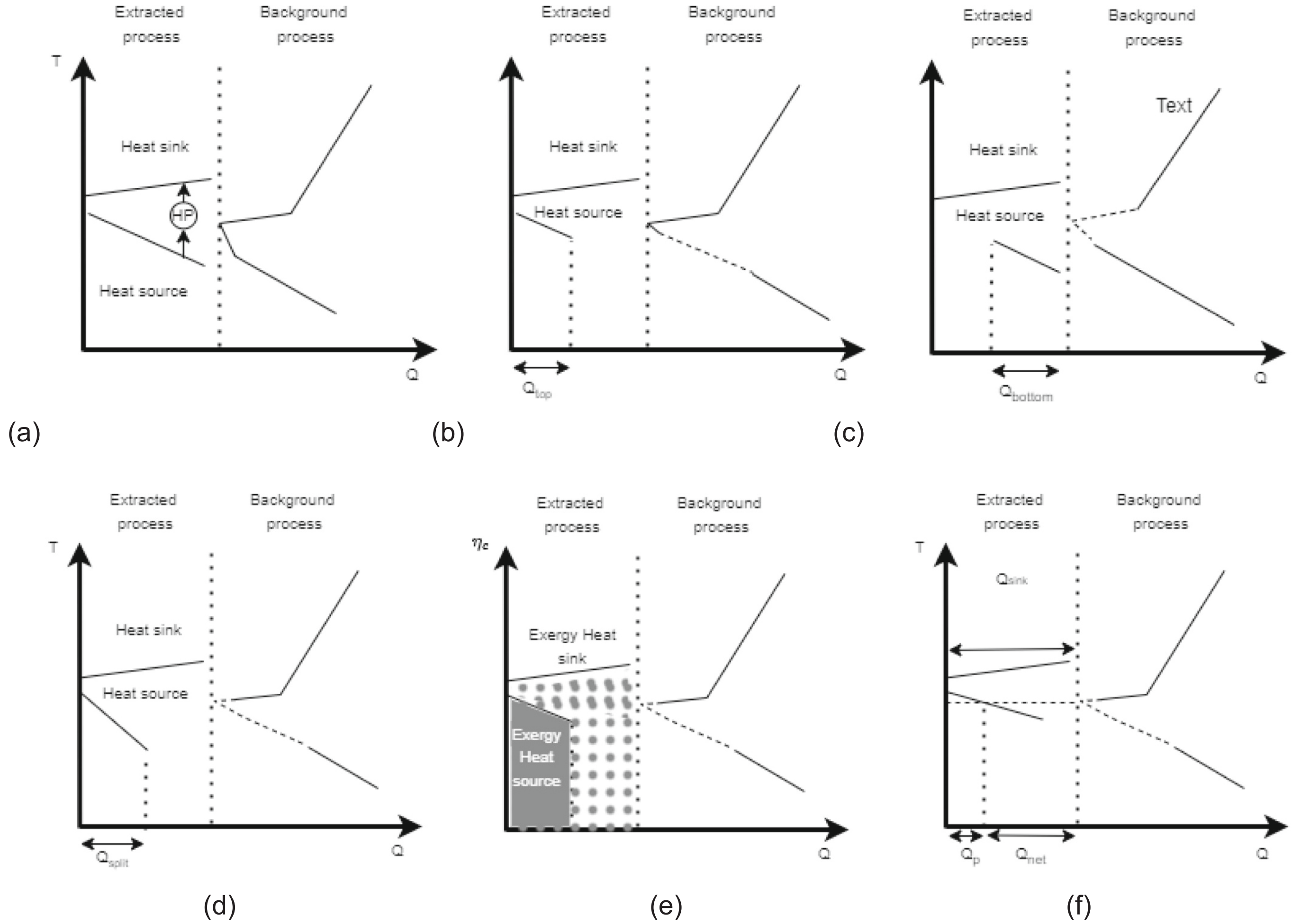

Fig. 1. Split grand composite curve. a) a split grand composite curve of a process where an extracted heat source is connected to an extracted heat sink by a heat pump, which transfers heat across the background process. b) is a split grand composite curve of the same process where a heat pump is extracted and only the top-end of the stream is used, but where the bottom-end is not and is transferred in the background process, forming the dotted line in the process. c) is a split grand composite curve of the same process, but with the bottom-end of the heat source connected to the heat pump and the top-end being transferred back into the background process, forming the dotted line in the process. d) is a split grand composite curve of the same process with a heat pump extracting heat across the entire temperature range (split integration) and transferring excess heat to the background process, forming the dotted line. e) Split - exergy grand composite curve of the same process, where the work potential of the heat source is marked by a solid line and the exergy requirements for the heat sink are marked with dots. f) a split grand composite curve of a process where a part of the heat (Q_p) is extracted above the background pinch temperature and is therefore not transferred across the background pinch point.

as the heat pump and its connections were assumed to be implemented first. The selection of process changes started at the pinch point, where heat integration is most constrained. Guided by the Split-GCC, process units that influence the pinch point were listed in a table. Possible alternative processes or synthesis routes were explored based on results found in literature. The project development and deployment time of the heat pump was assumed in the order of 2–5 years and its technical lifespan to be at 15 years. Furthermore, only technologies with a minimal technology readiness level (TRL) of 6 were considered as they were identified as possible technologies to impact the plant's heat integration.

The pinch temperature of the background process was altered by replacing processes that directly or indirectly form the pinch. The temperature should be increased when a heat pump (partially) extracted heat from above the pinch point of the background process. The opposite should occur when the heat pump (partially) delivered heat below the pinch point of the background process. An increase in the pinch temperature was realized by deploying process changes that increased the net heat available above the pinch point. This was either realized by increasing heat apparent in waste heat streams or by decreasing heat demand. Decreasing the pinch temperature was realized in the opposite manner.

2.3. *Assessment of the impact of process changes on the heat pump's COP*

Process changes do not necessarily reduce the COP of the heat pump itself but may likely affect its performance on a plant-level, due to penalties from inappropriate placement. The COP on a plant-level, also called the effective COP (COP_{eff}) of the heat pump, was defined based on the amount of heat transferred across the pinch of the background process (Q_{net}) and the work required to operate the heat pump, as in Eq. (4):

$$COP_{eff} = \frac{Q_{net}}{W_{comp}} \tag{4}$$

The penalty (Q_p) resulting from the inappropriate placement was defined as the difference between the

amount of heat delivered (Q_{sink}) by the heat pump and the amount of heat transferred across the pinch point of the background process (Q_{net}), as in Eq. (5), and as visualized in Fig. 1.f.

$$Q_p = Q_{sink} - Q_{net} \tag{5}$$

3. Process descriptions of the case studies

Most heat-related emissions stem from operating separation processes [1,22,23]. For this assessment, a biodiesel production plant in the North-West Europe was selected as an example of a process where heat integration is limited by a distillation column, characterized by an isothermal heat source and sink. This case study is used to show how exergy-extended PCA can be used to identify beneficiary process changes next to a heat pump. Additionally, a case study on the purification process of vinyl chloride monomer (VCM) in Scandinavia is included to provide insights into design choices when dealing with non-isothermal heat sources and sinks. This case illustrates how the deployment of the heat pump itself can affect the formation of the pinch point and its plant-level COP.

3.1. *Case 1: Biodiesel production unit in North-West Europe*

The transesterification process of vegetable oils for biodiesel production has been extensively documented in literature, see e.g., Van Gerpen [24] and Luna [25]. Fig. 2 illustrates the heating and cooling requirements of the various process stages assuming that the oil is fed at a rate of 25 t/h. Initially, the feed is heated from the environment conditions to 70 °C for the degumming process. Subsequently, the oil is further heated to 240 °C for deacidification. After neutralization, the oil feed is cooled and mixed with methanol in a reactor (Reactor 1) operating at approximately 65 °C to produce FAME (fatty acid methyl esters) and glycerol. A sedimentation tank (separator 1) is used to separate the glycerol from the FAME and unprocessed reactants. The FAME-rich stream containing unreacted reactants undergoes transesterification in a second reactor (Reactor 2) at 55 °C. The products from this reactor are once again separated in sedimentation tanks (Separator 2). By-products, contaminants, and excess methanol are neutralized and removed in a wet water washing column. The wet FAME stream is then dried to meet the desired product quality. Excess methanol, glycerol, and other compounds are directed to a methanol-recovery column. In this column, methanol is separated from the other products, with a reboiler temperature of 102 °C. The condensed top stream of 65 °C is recycled to the reactors along with fresh methanol. The bottom product, consisting primarily of glycerol and water, is dried in a multi-effect evaporator, where the first stage operates at 102 °C and subsequent stages utilize flash condensate. The evaporated water is reused in the wash column.

The heating requirements are summarized in Table 1, indicating the supply temperature (T_s), target temperature (T_t), heat capacity flow rate (CP), and heat load (Q).

3.2. *Case 2: Vinyl chloride monomer purification process in Scandinavia*

The separation process of Vinyl Chloride Monomer (VCM) from

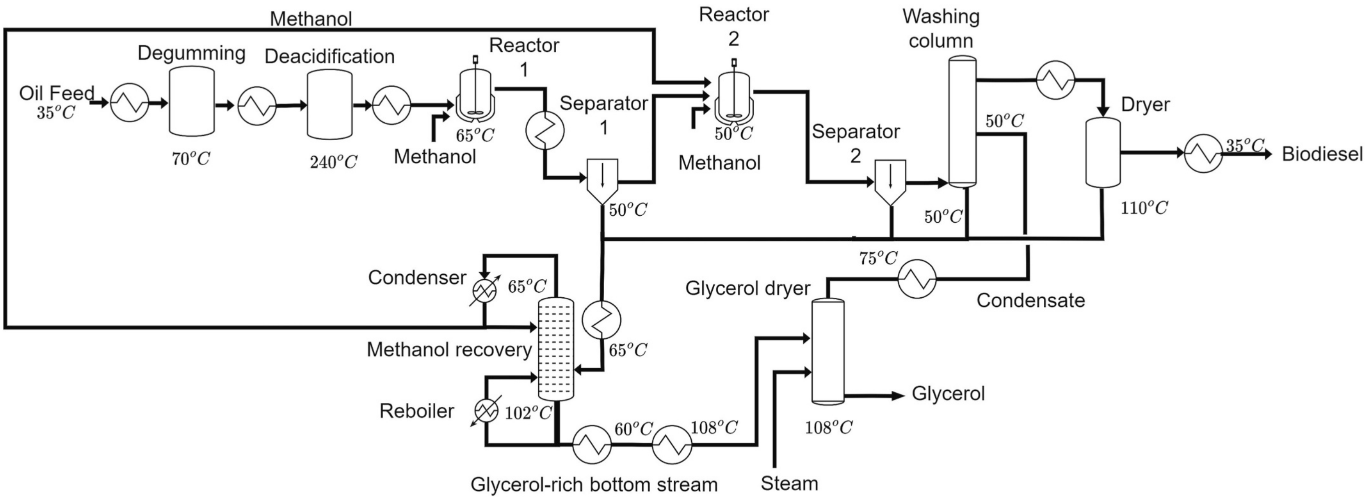

Fig. 2. Process flow diagram of the modelled biodiesel production process.

Table 1
Heating requirements of the biodiesel production process in North-West Europe.

Sub-process	Type	T_{supply}, °C	T_{target}, °C	CP, kW/K	Q, kW
Degumming	Cold	35	70	12.9	450
Deacidification	Cold	70	240	16.2	2750
Reactor 1 feed	Hot	240	65	15.4	2700
Separator 1 feed	Hot	65	50	10.0	150
FAME dryer preheat	Cold	50	110	15.0	900
FAME dryer	Cold	110	110	–	50
FAME cooler	Hot	110	35	15.0	1125
Column preheat	Cold	50	65	11.0	165
Reboiler	Cold	102	102	–	1850
Condenser	Hot	65	65	–	1550
(Reboiler) bottom cooler	Hot	102	60	5.5	230
Glycerol dryer preheat	Cold	60	108	5.5	265
Glycerol dryer	Cold	108	108	–	200
Glycerol condensate cooler	Hot	75	50	0.4	10
Glycerol cooler	Hot	75	35	1.8	70

ethylene dichloride (EDC) in a PVC production site in Sweden has been well documented by Lindqvist [26]. Fig. 3 illustrates the heating and cooling requirements of the various separation stages. Initially, the EDC is preheated from 27 °C to 207 °C and evaporated it at that temperature before the cracking process. Preheating between 125 °C and 193 °C was integrated with the cracker and therefore exempted from this study as the cracker is integrated with another production process. Thermal duties were based on a volume flow 45 m^3/h at 23 bar exiting the EDC plant. The first separation step after cracking removed tars from the mixture of VCM, EDC, hydrogen chloride (HCl), water and tars in a cooling column. Valuable products absorbed in the tar were separated in a distillation column, where the reboiler heats the tar from 90 °C to 141 °C. The top stream of the tar column was recycled back into the cooling column. The distillate of this column was condensed in three stages from 132 °C to 40 °C caused by a partial condensation of the stream's content. A mix of EDC, VCM and HCl was fed into the HCl column, where the reboiler operates at 87 °C and HCl was condensed at the top at −32 °C and sequentially evaporated until a temperature of 21 °C to comply with the process conditions set by connecting processes. The bottom stream consisting of VCM and EDC was heated and partially evaporated at 158 °C after which the VCM was condensed at 40 °C and brought back to environmental conditions. All heating requirements were summarized in Table 2, indicating the supply temperature (T_s), target temperature (T_t), heat capacity flow rate (CP), and heat load (Q).

4. Results

The result section consists of two parts, where the results of the study on the biodiesel case are presented in section 4.1, and those of the VCM case in section 4.2. In the biodiesel case study of section 4.1, the emphasis is on the impact of process changes on the heat pump's plant-level performance. The impact of deploying a heat pump on its plant-level performance itself is of lesser interest due to the heat pump's latent heat source and sink in the distillation column. This is not the case for the VCM-purification process, where the pinch is formed by sensible streams, which is the central theme of section 4.2.

Table 2
Process data table of the reference VCM separation process adapted from [26].

Sub-process	Type	T_s, °C	T_t, °C	CP, kW/K	Q, kW
EDC-preheat I	cold	27	125	20.2	1980
EDC- preheat II	cold	193	207	27.5	385
EDC-evaporator	cold	207	207	–	3045
Cooling column condenser A1	hot	132	112	−145.3	2905
Cooling column condenser A2	hot	112	66	−89.2	4105
Cooling column condenser B	hot	66	40	−80.8	2100
HCl-preheat	hot	40	13	−4.1	110
HCl-condenser	hot	−32	−32	–	1640
HCl-heater	cold	−32	21	2.1	110
HCl-reboiler	cold	87	87	–	1560
VCM-preheat	cold	82	85	153.3	460
VCM-condenser	hot	40	40	–	2500
VCM- subcooler	hot	39	17	−16.6	365
VCM-reboiler	cold	158	158	–	2210
Tar-reboiler	cold	90	141	3.5	180
Tar-condenser A	hot	92	85	−8.6	60
Tar-condenser B	hot	85	52	−1.7	55

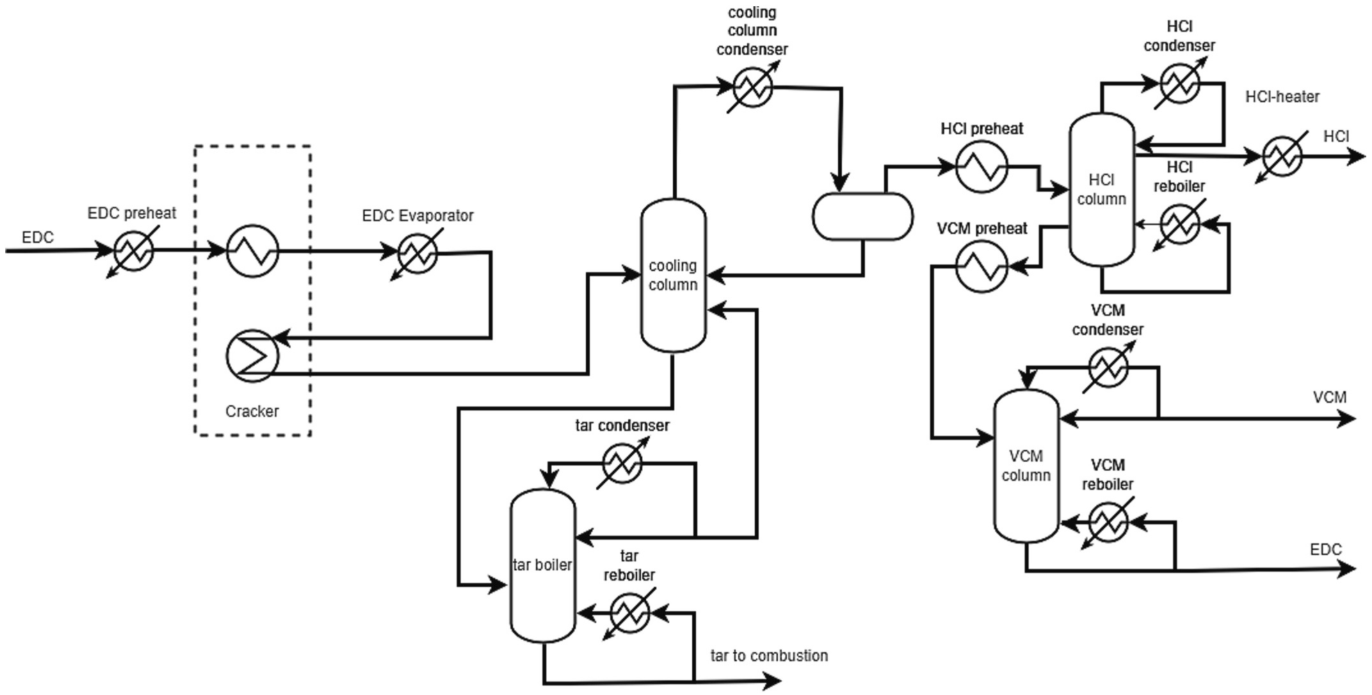

Fig. 3. Process flow diagram of the reference VCM separation process adapted from [26].

4.1. Case 1: Biodiesel production

The results of the biodiesel case are structured in accordance with the steps presented in the method section.

4.1.1. Selection of heat pump connections

The grand composite curve of the original process is presented in Fig. 4.a. The difference between net hot and cooling requirements resulted from the inability to recover heat from the FAME dryer and from not including minor streams like the waste streams of the deacidification process. From Fig. 4.a. it can be derived that the pinch is formed at a shifted temperature of 60 °C. Heating requirements are limited to 107 °C. At this temperature, the first stream (Q_{h1}) with a significant heating requirement (1.9 MW) is the reboiler of the methanol recovery column. The condenser of the column is situated at the pinch and has a cooling requirement (Q_c) of 1.6 MW. These streams are selected to be the connections to the heat pump, as they are the closest to the pinch point that meet the set criteria of representing at least 10% of the total heating requirements. Other heat requirements are at a comparable temperature, hence, overproduction of heat by the heat pump could, without significant losses in efficiency, be utilized in other processes. In total 2.6 MW (Q_h) is needed to operate the production plant, of which about 1.9 MW (Q_c) is emitted to the environment. Heat pump connections are extracted from the background process in the Split-GCC of Fig. 4.b, where the reboiler and condenser are depicted on the left side of the graph and the background process is depicted on the right. The graph shows that the extracted process operates above the pinch of the background process and that heating (Q_h) and cooling (Q_c) requirements are reduced to 0.9 and 0.4 MW, respectively, when a heat pump provides the utility requirements of the extracted process.

4.1.2. Selection of process changes

4.1.2.1. Selection criteria for process changes.

A comparison between the

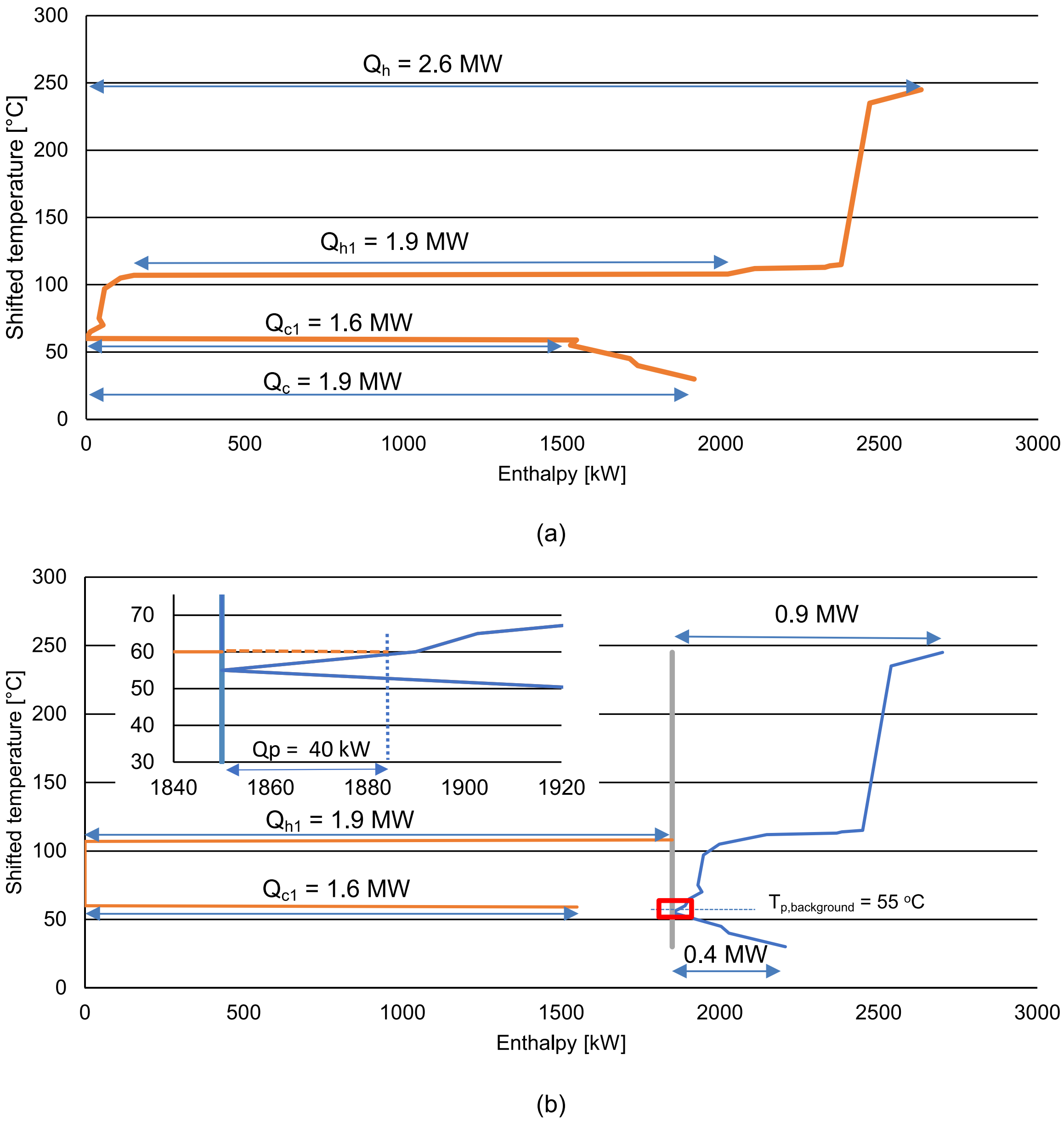

Fig. 4. Heat integration of the reference biodiesel production process: a) grand composite curve, b) split-grand composite curve with the heat pump connections extracted on the left side and the background process on the right. The operation of the heat pump above the background pinch point and the resulting deployment penalty is highlighted in the zoom at the top left of the graph.

extracted and background process in Fig. 4.b. shows that the shape of the grand composite curve is dominated by the methanol-recovery column, which is represented by the isothermal lines at a shifted temperature of 60 °C and 108 °C. Of the original 2.6 MW, only 0.9 MW of heat is required to operate the entire background process. The remaining 1.9 MW is needed to operate the reboiler of the methanol-recovery column. More importantly, the figure shows that the heat pump transfers heat above the pinch temperature of the background process at 55 °C. Hence, a heat pump that connects the streams in the extracted processes does not solely transfer heat across the pinch point of the background process. This inappropriate placement will lead to a penalty of 40 kW when all the condenser's heat is utilized by a heat pump [5,6], as depicted in the zoom in of Fig. 4.b. Its effective COP will therefore be lower than the COP of the heat pump itself. Process changes should therefore increase the temperature of the background pinch to at least 60 °C to avoid this loss. The temperature of the background pinch can be lifted by either reducing the cooling requirements and their temperature or by increasing heating requirements and their temperature just above the pinch.

4.1.2.2. Plausible process changes. The processes that release heat just above the pinch are listed in Table 3. Though the process of the bottom cooler provides heat until the shifted pinch temperature, it does not add to the amount of net heat available as the same amount of heat is required in the glycerol preheat at the same shifted temperatures. The same holds for the FAME cooler, which is integrated with the FAME preheat. This leaves the separator 1 feed cooler as the most dominant of other streams due to its larger heat capacity flow rate. The purpose of the separation feed cooler is to enable the separation process in the sedimentation tank [25]. Alternative separation methods could occur at higher temperatures and omit the need for this cooling step [27,28]. However, a similar heat exchanger would be necessary after the separation unit, as separation efficiencies of alternative technologies are comparable and the temperature requirements of the second reactor remain based on a chemical equilibrium with by-products [24]. Thus, the same amount of heat would become available after such a modification. Changes to the glycerol cooler could, however, reduce the net heat available just above the pinch as this process is not directly integrated with a preheater. The glycerol cooler and the rest of the drying step are required as the water added in the FAME purification process needs to be removed to bring the glycerol up to market conditions. Hence, exploring process changes to the FAME purification step, the wet water washing process, would therefore be a preferred route.

4.1.2.3. Process changes to the FAME purification step. A comparative study by Atadashi et al., [29] explored three technologies for purifying crude biodiesel: wet washing, dry washing, and membrane refining. In their comparison, they showed that using a membrane process would be the preferred option, as other technologies do not meet the required ASTM D6751 and EN14214 standards, which set requirements for biodiesel to be used as a fuel. Suthar et al. [30] confirmed these findings whilst searching for less energy-intensive separation technologies for biodiesel production. The process integration of a membrane process is depicted in Fig. 5. In this design, it is assumed that no additional heat is required to operate the membrane as the temperature of the stream after the second sedimentation tank is of the same order as the temperatures used in the biodiesel separation experiments by for example, Cao [27] and Dube [31]. The resulting process data table is presented in Table 4.

Table 3
Data of processes releasing heat just above the background pinch point.

Process	Type	Ts °C	Tt °C	CP kW/K	Q kW
Separator 1 feed	Hot	65	50	10.0	150
FAME cooler	Hot	110	35	15.0	1125
Bottom cooler	Hot	102	60	5.5	230
Glycerol condensate cooler	Hot	75	50	0.4	10
Glycerol cooler	Hot	75	35	1.8	70

4.1.2.4. Impact of process changes on the heat integration. The impact of replacing the wet water washer with a membrane separation unit on the grand composite curve of the background process is presented in Fig. 6. It shows that the pinch temperature of the background process increased to 97 °C and overall heat requirements (Q_h) in the background process were reduced to about 0.3 MW. Thereby, it shows that this modification not only helps in reducing heat-related CO_2 emissions but also increases the performance of the heat pump as it now operates across the pinch of the background process. Also note that the net excess of heat produced by the heat pump will increase if the duty in the heat pump's source is not lowered, as the required duty by the reboiler (Q_{h1}) will fall by about 150 kW to 1.7 MW. Moreover, deploying the heat pump will, therefore, no longer come with an inappropriate placement penalty, as the heat pump solely transfers heat across the pinch point of the background process. Net cooling requirements are reduced to near zero.

4.1.3. Assessment of the impact of process changes on the heat pump's COP

The Split-EGCC of the original production plant layout and the layout after the deployment of the membrane process are depicted in Fig. 7.a. and Fig. 7.b., respectively. Fig. 7.a. shows that in the original production plant, the heat sink holds an exergy value of 450 kW, whereas the source has only 180 kW available. Hence, together with an exergetic efficiency of 0.59, about 0.5 MW is required from the heat pump. The heat sink requires 410 kW after the deployment of the membrane due to the reduced water content in the column feed. The exergy available at the source is reduced to 170 kW. As a result, the required shaft work by the heat pump is reduced to 0.4 MW due to the reduced water content in the feed stream of the column. The heat pump was able to transfer 1.9 MW of heat in the original layout with a penalty of 40 kW (as seen in Fig. 4.b.), which brings it near 1.8 MW, resulting in an effective COP of 4.0. After deploying the membrane separation process, 1.7 MW of heat could be effectively transferred with a COP of 4.1, as the thermal duty of the reboiler was reduced. In this case, 0.3 MW remains unutilized at the heat source.

4.2. Case 2: Vinyl Chloride Monomer purification process

For the VCM case, only the impact of the deployment of the heat pump itself on the heat integration of the background process is explored. The impact of deploying other decarbonization technologies is not included to emphasize the role of heat extraction, and thereby the role of heat pump placement.

4.2.1. Extraction of heat pump connections

The grand composite curve of the reference model is presented in Fig. 8.a. The process requires 5.8 MW of heat (Q_h) and 7.6 MW of cooling (Q_c) to operate. The additional 0.8 MW of cooling is a result of the sub-ambient requirements of HCl. The pinch of the process forms at 127 °C as heat from the cooling column cannot be used to meet the demand of the tar-reboiler and the EDC-preheat. However, heat from the cooling column's condenser defines the shape of the curve just below the pinch, as it is the stream with the largest heat capacity flow rate from a shifted temperature of 127 °C to 105 °C. Hence, it is selected to be the heat source (Q_c) for the heat pump. The VCM-reboiler is selected to be the sink of the heat pump (Q_h), as it is the first stream that has at least 10% of the total heating requirements above the pinch at a shifted temperature of 163 °C. However, the condenser surpasses the thermal duty of the VCM-reboiler, 2.9 MW vs. 2.2 MW, respectively. This imbalance is also visualized in the Split-GCC (Fig. 8.b). As a result, not all energy from the condenser could be utilized in the reboiler. Hence, either the top, the bottom, or a split of the hot stream should be utilized.

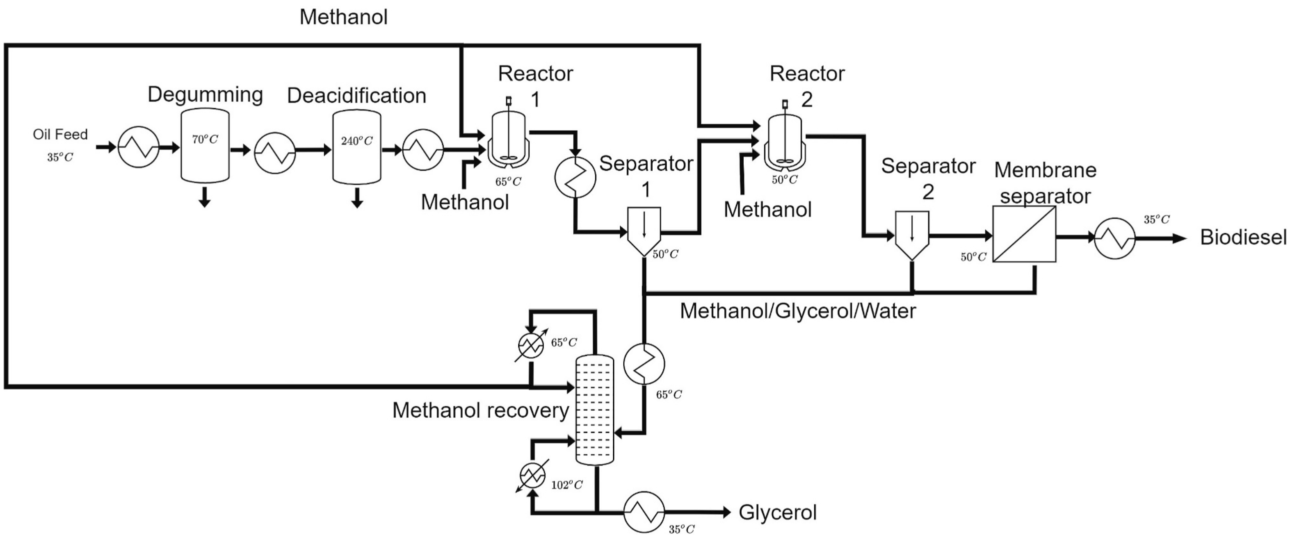

Fig. 5. Process flow diagram of the biodiesel production process after deployment of the membrane separation unit.

Table 4

Process data table of the biodiesel production process after deployment of the membrane separation unit based on the experiments of Cao [27] and Dube [31].

Sub-process	Type	T_s, °C	T_t, °C	CP, kW/K	Q, kW
Degumming	Cold	35	70	12.9	450
Deacidification	Cold	70	240	16.2	2750
Reactor 1 feed	Hot	240	65	15.4	2700
Separator 1 feed	Hot	65	50	13.3	200
Column preheat	Cold	50	65	3.3	50
Reboiler	Cold	102	102	–	1700
Condenser	Hot	65	65	–	1550
Bottom cooler	Hot	102	35	1.9	130

4.2.2. Selection of process changes

4.2.2.1. Top-end heat pump integration. The heat pump must deliver 2.2 MW of heat (Q_h) at a shifted temperature of 163 °C from a sensible 132 °C heat source with a capacity flow rate of 145 kW/°C. At this temperature, the sink has an exergetic value of 750 kW. Solving the energy balance and estimating the heat pump's COP with Eq. (1–3) indicates that the source should be cooled by 1.6 MW (Q_c) to 121 °C, with an exergetic value of 430 kW. Both energy and exergy values are presented in Fig. 9.b. Fig. 9.a. The compressor needs 0.57 MW to overcome the difference in exergy, as presented in Table 5. Fig. 9.a. shows the impact on the background process of reverting the excess energy of the heat source back into the background process. As a result, the pinch point of the background process is formed at a shifted temperature of 116 °C. This is below the pinch that is formed by the heat pump between a shifted temperature of 158 °C and 127 °C. This inappropriate placement comes with a penalty of 0.26 MW.

4.2.2.2. Bottom-end heat pump integration. As with the top-end integration, the heat pump must deliver 2.2 MW (Q_h) at a shifted temperature of 163 °C from a sensible heat source with a capacity flow rate of 145 kW/°C. However, in this scenario 1.5 MW is extracted (Q_c) between 123 °C and 112 °C. At these temperatures, the heat sink and source have an exergy value of 400 kW and 750 kW, respectively. Hence, with an exergetic efficiency of 59%, 0.65 MW is required by the heat pump, as presented in Table 5 and Fig. 9.d. Fig. 9.c. shows that the heat pump transfers heat entirely across the pinch point of the background process at a shifted temperature of 127 °C. As a result, the heat pump faces no inappropriate placement penalty.

4.2.2.3. Split heat pump integration. The heat capacity flow rate of the heat pump's heat source must be reduced to deliver the requested 2.2 MW at the heat sink (Q_h). The split stream set-up utilizes the entire

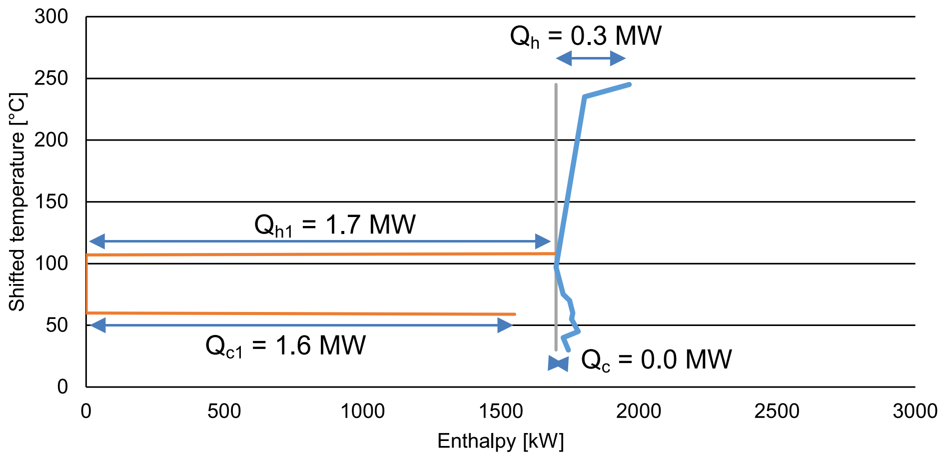

Fig. 6. The split grand composite curve of the biodiesel production process after deployment of the membrane separation unit, where the heat pump connections are extracted (left) from the background process (right).

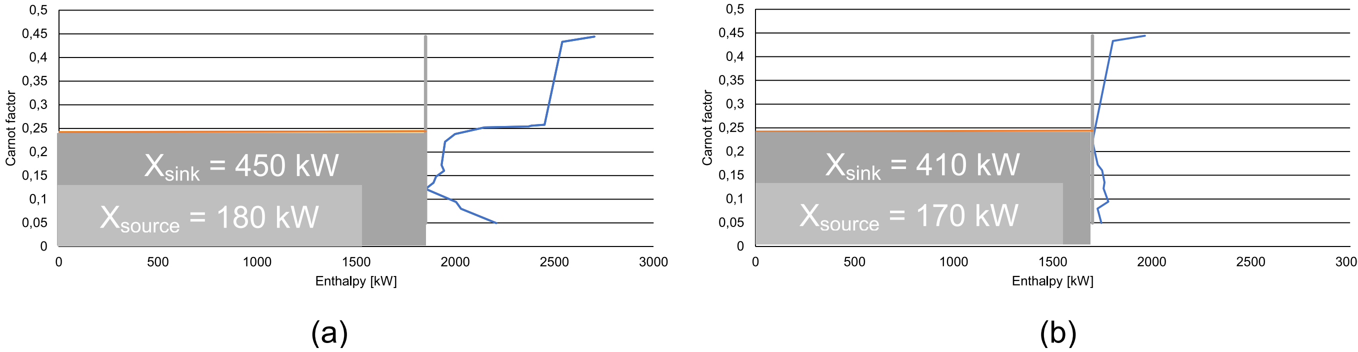

Fig. 7. Split exergy grand composite curves of: a) the original biodiesel production process, b) the biodiesel production process after deployment of the membrane separation unit.

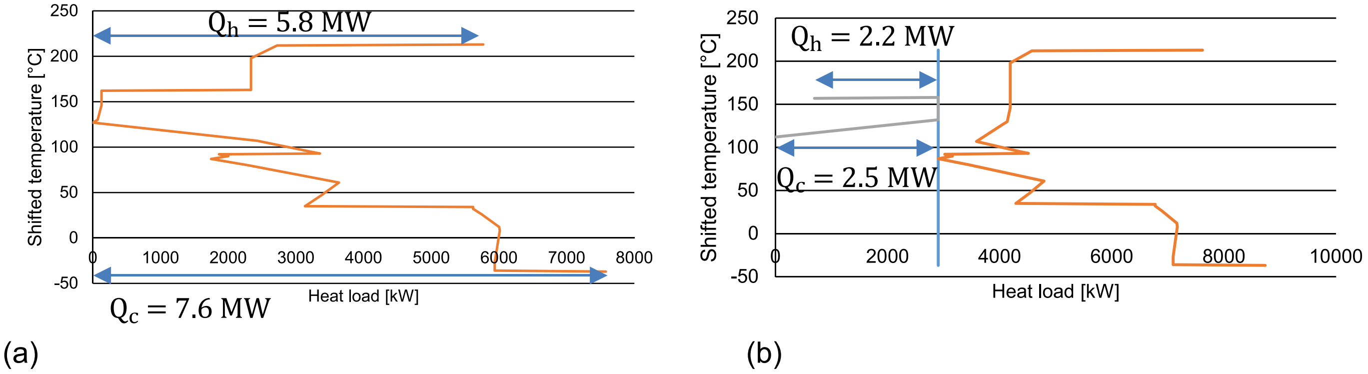

Fig. 8. Heat integration of the reference Vinyl Chloride Monomer purification process: a) grand composite curve, b) split-grand composite curve with the heat pump connections extracted on the left side and the background process on the right.

temperature range from the heat source, 132 °C to 112 °C. The heat pump requires 0.61 MW to overcome the exergy difference between the sink (750 kW) and the source (390 kW). 1.6 MW (Q_c) is required from the heat source by the heat pump, as presented in Table 5 and Fig. 9.f. This is realized by creating a stream with a capacity flow rate of 80 kW/°C. The impact of reverting the excess energy of the heat source back into the background process is shown in Fig. 9.e. Due to this change, the heat pump is appropriately placed across the pinch point of the background process at a shifted temperature of 127 °C and faces no penalty.

4.2.3. *Assessment of the impact of integration strategy on the heat pump's COP*

The top-end heat pump integration reduces the process heat requirements by from 5.77 MW in the reference case by 1.9 MW to 3.82 MW, as can be seen in Table 5. This 0.3 MW less than the 2.2 MW that is delivered at the heat pump's sink. This difference is due to the inappropriate placement penalty as the heat pump partially operates above the pinch point of the background process, as shown in Fig. 9.a. The other two options transfer heat entirely across the pinch (see Fig. 9.c. and 9.e). However, due to the lower exergy value of the heat sources, these two options require more work from the compressor, which results in a penalty in the form of additional exergy destruction. As a result of this trade-off between a heat and work penalty, the net COP of the Top-end and Bottom-end heat pump integration are quite comparable, with a COP of 3.45 and 3.41, respectively. The split heat pump integration, however, can transfer heat without facing a penalty and maximize the work potential of the heat source and come to a net COP of 3.63, resulting in an overall increase of 6.5% compared to the top-end approach.

5. Discussion

Both cases were selected because of their limited complexity to clearly demonstrate how process change analysis (PCA) can be used to identify how process changes will impact a heat pump's performance. However, the layout of the biodiesel production unit, consisting of a set of reactors and sequential separation processes, is typical for a large part of the industrial sector. Just as the heat integration is being dominated by a single separation step, as is also the case in, for example, a paper mill [32]. However, the vinyl chloride monomer (VCM) purification case also illustrated how to apply the method in case multiple processes form the pinch point. Challenges may arise when considering highly complex plant layouts, as upstream changes may have unforeseen impacts on the energy and mass balance, and thus the heat integration, further down the line.

Another dimension of complexity is the use of multiple heat sinks or sources, though a single sink-source system is commonly the most cost-effective strategy [10]. A possible exception to this is the case where low-pressure steam is being produced for the heat sink with the lowest temperature and excess steam is being (re)compressed to supply heat to higher temperature sinks. This added complexity requires heat extraction/delivery strategies akin to that of the VCM-case but include the extraction of additional streams. The use of multiple heat sinks is a likely improvement for the biodiesel case, where other relatively large heat sinks are apparent close to the reboiler, and the condenser still has 0.1 or 0.3 MW of heat left respective of the reference or the altered case. This energy should be transferred back to the background process, as is demonstrated in the VCM-case, when this energy is not utilized. This heat will help avoiding the 40 kW penalty incurred in the case of the reference process. This cancellation will always occur when the amount of excess heat in the heat source exceeds that of the heating

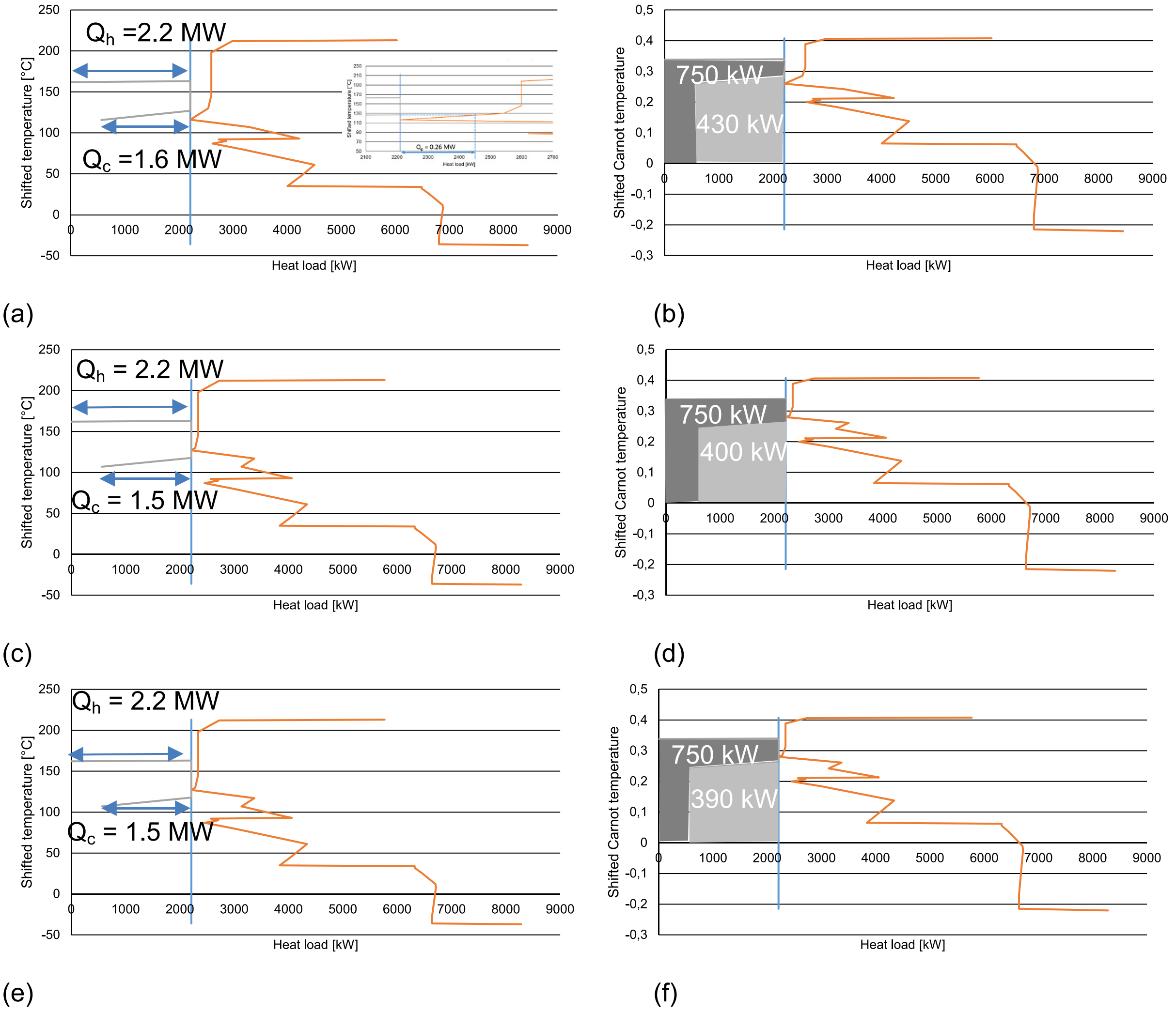

Fig. 9. Heat integration profiles: a) grand composite curve in case of top-end heat extraction, b) exergy grand composite curve in case of top-end heat extraction, c) grand composite curve in case of bottom-end heat extraction, d) exergy grand composite curve in case of bottom-end heat extraction, e) grand composite curve in case of split heat extraction, f) exergy grand composite curve in case of split heat extraction.

Table 5
Comparison of heat extraction strategies for heat pump implementation.

	Process heat [MW]	Energy source [MW]	Exergy source [MW]	Work target [MW]	Work required [MW]	Exergy destruction [MW]	Net energy consumption [MW]	COP_{nett}
Reference	5.77						5.77	
Top-end	3.82	1.65	0.46	0.33	0.57	0.23	4.38	3.45
bottom-end	3.56	1.56	0.41	0.38	0.65	0.27	4.21	3.41
split	3.56	1.60	0.43	0.36	0.61	0.25	4.17	3.63

requirements at the same shifted temperature in the background process.

Another potential challenge is the formation of a new pinch point by a “near pinch” resulting from a large heat integration pocket. This scenario was not included in the cases, but there are no fundamental barriers that would not allow for the use of PCA with the split (exergy) grand composite curve (Split-(E)GCC) when this is the case. The formation of the new background process pinch point would be clearly visible in a Split-EGCC, which would allow for appropriate integration of the heat pump and help to identify process changes that modify the background pinch point in a similar way as for the original pinch point. Additionally, “pocket-heat pumps” also could be used to overcome this challenge [33]. The same argument holds for processes where a larger inappropriate placement penalty is encountered.

However, it should be noted that in its current form the approach is limited to continuous steady-state processes. It is not suited for discontinuous processes, e.g., batch processes, and should be expanded with methods like the time-slice model of floating pinch analysis to cope with this complexity [7].

A practical drawback to the approach is its abstract representation of a process, as is inherent to pinch analyses, making it difficult to communicate results to non-experts, like financial decision makers. It is, therefore, advised to use this approach as an exploratory tool and communicate results via conceptual designs based on the results.

6. Conclusions

Process Change Analysis (PCA) extended with the split- exergy grand composite curve (split -EGCC) proved to be a valuable tool in assessing the impact of process changes on the performance of a heat pump. In the biodiesel production process, it showed that when a heat pump transfers heat between the condenser and the reboiler of the methanol recovery column it faces an inappropriate placement penalty of 40 kW. PCA helped to identify which processes caused this penalty and how it could be avoided whilst reducing the process's overall heat requirements. This was achieved by replacing the wet water washing column with a membrane separation unit. The deployment of this unit resulted in a reduction of heating requirements from 0.9 MW to 0.3 MW, whilst increasing the plant-level COP from 4.0 to 4.1.

Furthermore, PCA effectively identified the optimal utilization of a sensible heat source in the vinyl chloride monomer (VCM) process. Extracting heat from the top-end minimized work requirements by leveraging the steam's high exergy value but led to an inappropriate heat pump placement penalty. Utilizing bottom-end heat avoided this penalty but resulted in higher work requirements due to the streams lower exergy content. Splitting the heat source achieved the highest plant-level COP. Overall, this strategy yielded a deviation of over 6.5% in COP values. These findings underscore the importance of strategic heat extraction to optimize heat pump performance.

Further research needs to determine how PCA can include the temporal aspects of heat sources and sinks to accommodate process fluctuation and those demanded by the energy system.

Overall, the results underline the importance of the combined assessment of process changes, stream selection, and heat integration technologies by highlighting the effect process changes have on the performance of a heat pump. PCA can, therefore, be a valuable tool in a period of continuous retrofitting that will include technologies, like heat pumps.

Nomenclature

Letter symbols

CC	Composite curve
COP	Coefficient of Performance
CP	Heat capacity flow rate, kW/K
Split-EGCC	Split exergy grand composite curve
GCC	Grand composite curve
Q	Stream heat load/ heat, kW
T	Temperature, °C
Split-GCC	Split grand composite curve
X	Exergy, kW

Greek symbols

η	efficiency

Subscripts and superscripts

0	environment
c	Carnot
trans	transferred
net	net
p	penalty
pl	plant-level
source	heat source
sink	heat sink
s	source
t	target

Disclosure

During the preparation of this work the author(s) used ChatGTP3.5 in order to improve readability and flow of the text. After using this service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

CRediT authorship contribution statement

Brendon de Raad: Writing – review & editing, Writing – original draft, Visualization, Validation, Resources, Project administration, Methodology, Formal analysis, Data curation, Conceptualization. **Marit van Lieshout:** Writing – review & editing, Supervision, Resources, Conceptualization. **Lydia Stougie:** Writing – review & editing, Supervision, Conceptualization. **Andrea Ramirez:** Writing – review & editing, Supervision, Conceptualization.

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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