Comparison of VCHP and MVR assisted distillation of MEG-water mixture via dynamic simulations

Tyraskis I. [a], Sarić M. [a], Marina A. [a], Padberg P. [b], Gräber M. [b], Pellny Y. [b]
[a] TNO, 1755 ZG, Petten, the Netherlands
[b] TLK Energy GmbH, 38106 Braunschweig, Germany
ioannis.tyraskis@tno.nl

Abstract. Tackling the energy efficiency of distillation holds the promise of the largest energy savings potential, as it is recognized as the most energy intensive operation in the chemical industry, while also presenting poor efficiency. Although the process consumes a considerable amount of heat, it also rejects it at a lower temperature. In the current project, we study the utilization of the waste heat in mono-ethylene glycol (MEG) dehydration column via dynamic simulations in Modelica software.

Two different concepts to perform the heat integration of MEG dehydration were evaluated and compared in terms of energy savings and process control: Vapor compression heat pump (VHCP) and Mechanical vapor recompression (MVR). Both systems were studied in two different heat integration scenarios. The first scenario of "partial" heat integration considered about half of the total heat requirement to be supplied at intermediate stage(s) in a falling-film column configuration, at a temperature considerably lower than that of the reboiler. The remaining heat was supplied by an external source and was used to control the bottom stream purity. In the second scenario of "full" heat integration, both concepts were used at their full potential, thus maximizing heat integration with the reboiler. The control response of both systems was tested by introducing a feed concentration step of 2%.

The total specific energy use in the "partial" integration was comparable between the two configurations, resulting in 42% reduction compared to the conventional column. In "full" integration, the MVR was proved significantly more efficient, resulting in 41% specific energy reduction over the VCHP system, and 76% compared to the conventional column. The "full" heat integration concept resulted in more complicated designs and slow response in the MEG step. In order to achieve sufficient control of the product purity, a small percentage of external heat supply is essential.

Keywords distillation, heat pump, mechanical vapor recompression, falling-film, dynamic simulation

Introduction

The chemical industry is responsible for about one third of the total energy used in the industrial sector. Tackling the energy efficiency of distillation holds the promise of the largest energy - and the associated CO_2 emissions - savings potential, as it is recognized as the most energy intensive operation in the chemical industry accounting for 40% of total energy use [1], while also presenting poor efficiency [2]. The process requires a considerable amount of heat input, which it also rejects at a lower temperature. In the current project, we study the upgrade of the discharged waste heat and its re-use to reduce the utility consumption in the process. For this purpose, two different heat pump configurations are evaluated and compared:

1. Vapor compression heat pump (VHCP): Indirect heat pumping using a closed cycle with pentane as the working fluid.
2. Mechanical vapor recompression (MVR): The process fluid exiting the top of the column can be used as the heat pumping fluid for vapor recompression. In the current study, the top fluid is water (steam).

Both heat pump concepts require the input of electrical energy. Due to the uptake of waste heat at the lower temperature level, the heat produced by the heat pump exceeds the electrical input by a factor known as the coefficient of performance ($COP = Q_{heatpump}/W_{electrical}$). The achievable COP from the heat pump reduces as the required temperature lift increases.

The reference process simulated is the dehydration of mono-ethylene glycol (MEG). This process can be found in several application like (bio-)MEG production, Terephthalic acid production and MEG recovery for use as a hydrate inhibitor in Natural Gas production. The fundamental difference between applications is the feed and product specifications. As a reference case, the dehydration of a 36 mole% MEG stream up to 85 mole% is considered, which is relevant to all the aforementioned processes. The technical characteristics of the conventional process can be seen in Figure 1, where a falling-film distillation column is considered. A falling-film configuration enables steam supply (at a lower temperature than needed in the reboiler) across the trays of the column, but does not affect the total heat demand of the distillation process. Figure 1 shows an energy and mass balance of the reference process.

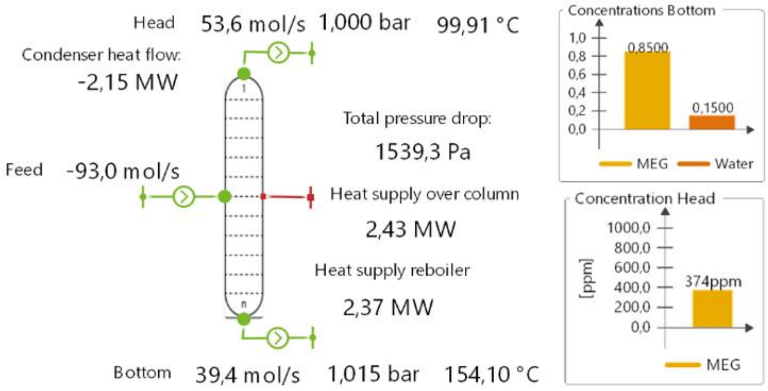

Figure 1: Falling-film distillation base case. Approximately half of the heat needed is supplied across the column using a heat chamber. This does not affect the energy consumption, which is similar to supplying the all the heat in the reboiler. Green lines indicate mass transfer, and red lines indicate heat transfer.

Simulations

The models presented in this study were developed using Dymola software, which is based on Modelica object oriented language, in combination with the commercial TIL and PSL library by TLK Thermo and TLK Energy[3]. Additionally, the KBC Multiflash software was integrated to the simulation in order to extract the thermodynamic properties of the MEG-water mixture [4]. The distillation column is modelled using stages with fixed volumes including varying pressure and vapor hold-up. For each stage an equilibrium is calculated using UV-flash. The mass transfer between stages is pressure-driven and the heat transfer into stages is assumed ideal. Steady state analysis shows results are in agreement with more commonly used ASPEN software. The heat pump models utilized vary in level of included physical features. Relative complexity of the VCHP is high (physical based) whilst for the MVR it is low (efficiency based - 70% isentropic), however both models are representative of performance that could be expected to be achieved in practice.

The VCHP and MVR configurations are analyzed for two different concepts:

1. Partial heat integration: Supply the upgraded heat to the column stages, and not to the reboiler, in order to reduce the temperature lift and maximize the COP. This is a viable option in the MEG-water separation, because of the high difference in relative volatilities of the components which results in significant temperature difference between the last column stage and the reboiler (~30 ºC). The heat is supplied to the whole column or to the last stage(s) using a falling film configuration, where the distillation column is placed inside a steam chamber and the upgraded steam is supplied from the top. Such configuration is present in TNO lab.
2. Full heat integration: Supply the upgraded heat to the reboiler. This concept minimizes the external heat supply to the process, but also lowers the COP of the heat pump, since the temperature lift is higher. The small amount external heat can be supplied at an intermediate stage of the column.

Both concepts are analyzed for the two heat pump configurations , thus forming 4 scenarios:

1a. VCHP “partial” heat integration that supplies part of the available heat to the column
2a. VCHP “full” heat integration that supplies all available heat to the reboiler
1b. MVR “partial” heat integration that supplies part of the available heat to the column
2b. MVR “full” heat integration that supplies all available heat to the reboiler

All the scenarios were compared in terms of energy consumption (electricity and heat in steady state) and system control (dynamic response). The control was tested by introducing a 2% MEG concentration increase in the feed stream and measuring the response time in top and bottom product streams. The concentration step occurs at 20000s of simulation time. 1a and 1b scenarios use 93 mol/s feed flow, whereas 2a and 2b scenarios use 47.7 mol/s. The higher feed flow is needed for the 2a scenario to match the heating capacity of a (complex) pre-existing VCHP system model. It was also used in 2b to allow direct comparison with 2a. In any case, all scenarios can be fairly compared with each other by calculating the energy per mol of product.

Regarding the VCHP simulation, in scenario 1a (see Figure 2 Left), the column condenser acts as the source for the evaporator of the heat pump whereby partial condensation of the distillate occurs, and the condensate is recycled back to the column. In 2a (see Figure 2 Right), at least 70% of the distillate needs to be condensed, which means that liquid distillate exits the column among with the vapors. In each case, the product purity is not affected, and the operation mode of the condenser can be total or partial, provided that the feed stream enters at the middle of the column.

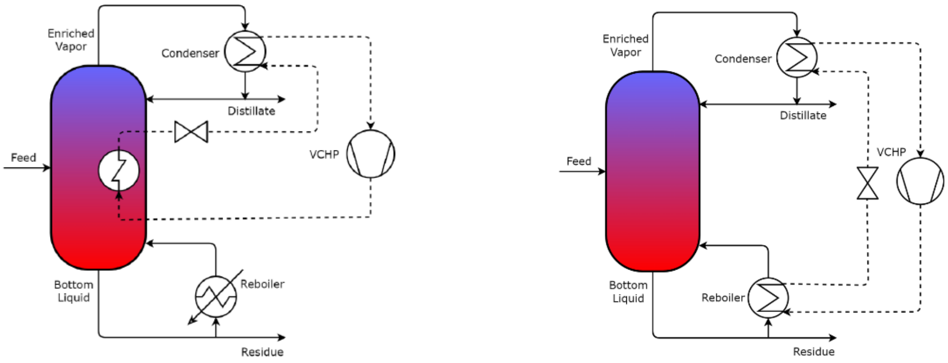

Figure 2: Schematic illustration of VCHP configurations. The heat pump delivers heat to the steam chamber across the column (scenario 1a-Left) or the reboiler (scenario 2a-Right).

Regarding the MVR, in 1b scenario, a partial condenser is considered. This means that either the vapor distillate of the partial condenser enters the compressor and is used for heating the column (Figure 3 Left), or that all the vapor exiting stage 1 enters the compressor and the distillate exiting the falling film chamber is recycled back to the column (Figure 3 Middle). In the current study, the former configuration is selected due to simplicity. In 2b scenario, all the vapors exiting stage 1 need to be condensed at the bottom reboiler after compression, so a total condenser is required (Figure 3 Right). Similarly, to VCHP configurations, this will not alter the results, provided that the feed enters at the middle stage of the column.

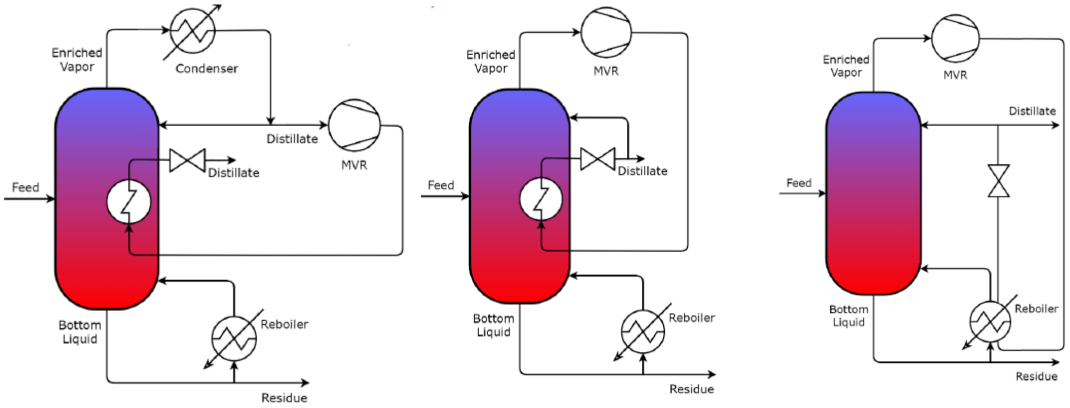

Figure 3: Schematic illustration of MVR configurations. The vapors exiting the partial condenser enter the compressor (Left). The vapors exiting stage 1 are compressed and the heat exchange across the column acts partial/total condenser (Middle). The vapors exiting stage 1 are compressed and the heat exchange in the reboiler acts as total condenser (Right).

The control strategy is the same in both VCHP scenarios, and it is performed using PI controllers:

- Liquid level in the reboiler is controlled through mole outlet of bottom product.
- Mole fraction at the bottom outlet of the column is controlled through the heat flow in the reboiler.
- Pressure in the condenser is controlled through mole outlet of the distillate.
- Mole fraction at the head outlet of the column is controlled through the speed of the compressor.

The control strategy for MVR scenarios is performed using PI controllers as well but it slightly differs between the scenarios. In 1b, the vapor distillate of the partial condenser enters the compressor (as shown in Figure 3 Left), whereas in 2b, the vapor exiting stage 1 enters the compressor (as shown in Figure 3 Right). This impacts the concentration control of the top distillate. In 1b, the distillate mole fraction is controlled by the condenser duty, whereas in 2b it is controlled by the reflux ratio.

The rest of the control strategy is the same in both MVR scenarios:

- Filling level in the reboiler is controlled through the mole flow at the bottom
- Mechanical input of the compressor controls the pressure in the column condenser
- Superheating downstream of the compressor is controlled through upstream liquid water inlet

Results

VCHP

Scenarios 1a and 2a are modeled according to Figure 2 Left and Right, respectively. In 1a, the heat pump is connected to the steam chamber of the column, whereas in 2a, the heat pump is connected to the reboiler. The heat pump model remains exactly the same for both scenarios, and the feed flow of 2a is adjusted in order to fit the capacity of the heat pump. The steady state results of the simulations are presented in Table 1.

Table 1: Steady state results of VCHP simulations in 1a and 2a scenarios.

Scenario 1a	Scenario 2a
VCHP T_{evap} = 95 °C, ΔT = 5K (Column $T_{condenser}$ =100 ºC)	VCHP Tevap = 95 °C, ΔT = 5K (Column $T_{condenser}$ = 100 ºC)
VCHP T_{cond} =128 °C, (Column T_{stage_5} =118 ºC)	VCHP Tcond=159 °C, Column $T_{reboiler}$=154 ºC)
ΔT_{lift} = 33 ºC	ΔT_{lift} = 64 ºC
$Q_{heatpump}$ = 50.6 % of total	$Q_{heatpump}$ = 97.2% of total
$Q_{reboiler}$ = 49.4% of total needed at 159 ºC	$Q_{external}$ = 2.8% of total needed at 123 ºC
COP = 5.2	COP = 2.6

The temperature lift is lower for scenario 1a, which results in higher COP. However, the available heat can only cover half of the column requirements, which means the process requires external heat supply at 159 ºC. On the other hand, 2a only needs 2.8% external heat, which can be supplied at 123 ºC. The response times to return to the product steam specification after the feed concentration step are shown in Figure 4 for 1a (Left) and 2a (Right). Both scenarios show adequate response times and can reach steady state using PI controllers. 1a needed 3 min and 70 min, while 2a needed 10 min and 30 min to correct top and bottom MEG concentrations respectively. Controller parameters were not optimized in this study, meaning that response times can likely be significantly improved.

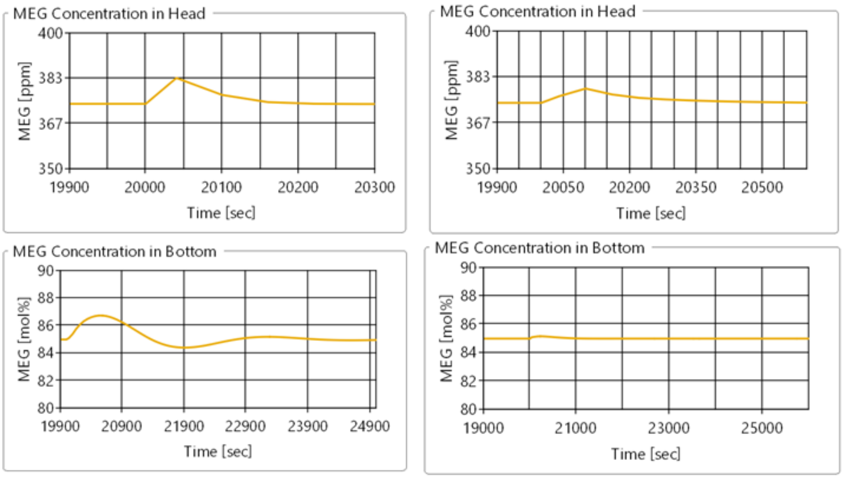

Figure 4: Response times for 1a MEG concentration in head (Top-Left) and bottom (Bottom-Left). Response times for 2a MEG concentration in head (Top-Right) and bottom (Bottom-Right).

It was attempted to eliminate the $Q_{reboiler}$ in scenario 2a, as it was technically possible to supply the whole heat demand via the heat pump. However, this complicates the control structure, as the controllers for the concentration at the column head and bottom, now, both influence the heat transfer from the column condenser to the HP evaporator. The resulting control response is slow and the system does not fully reach steady-state. It might be possible to control the system with more in-depth analysis, but total lack of external heat definetely increases the complexity and the response times.

MVR

The models of 1b and 2b scenarios were described in Figure 3-Left and Figure 3-Right respectively. Now, they are also shown in Figure 5, Left and Right respectively, in the more detailed Dymola environment where PI controllers and sensors are included. The results of the simulations are presented in Table 2.

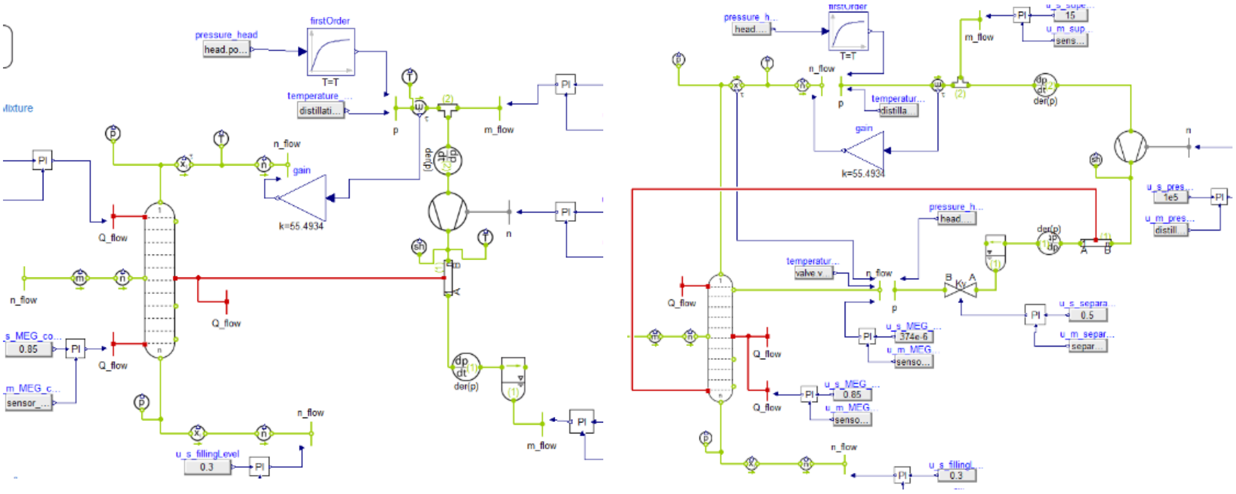

Figure 5: Schematic illustration of the MVR models of the 1b scenario (Left) and 2b scenario (Right), as shown in Dymola. Separate streams were used to connect the column head with the MVR inlet and outlet streams for simplicity. A separator is used after the heating tube in order to set the tube pressure and ensure that the whole gas is condensed inside the tube.

Table 2: Steady state results of MVR simulations in 1b and 2b scenarios.

Scenario 1b	Scenario 2b
Column $T_{condenser}$ = 100 °C	Column $T_{condenser}$ = 100 °C
MVR T_{cond} =140 °C, (Column Tstage_5=118 °C)	MVR T_{cond} =172 °C, (Column $T_{reboiler}$ = 154 °C)
ΔT_{lift} = 40 °C	ΔT_{lift} = 72 °C
Q_{MVR} = 47.2 % of total	$Q_{heatpump}$ = 94.1% of total
$Q_{reboiler}$ = 52.82% of total needed at 159 °C	$Q_{external}$ = 5.9% of total needed at 123 °C
COP = 10.8	COP = 5.2

Similarly to the VCHP simulations, the temperature lift is lower for scenario 1b, which results in higher COP. However, the available heat can only cover half of the column requirements, which means the process is dependent on external heat supply at 159 °C. Scenario 2b needs only 6% external heat, which can be supplied at 123 °C, but it is impossible to be completely eliminated as in VCHP configuration of 2a. The control strategy used in 1b controls the distillate mole fraction is by manipulating the condenser duty, which regulates the condenser's temperature. The simulation requires 3 min to correct distillate purity and 80 mins to correct bottom product purity after the step. These response times are similar to the results of 1a scenario. On the other hand, 2b control structure is not able to reach steady state. Here, a PI controller is used to manipulate the reflux ratio, which results in slow response times, thus requiring further optimization by more complicated control strategies.

Comparison of performance of all cases

Table 3 summarizes the performance of all scenarios. The "partial" integration scenarios show similar performance and both achieve approximately 42% reduction of total energy requirements compared base case distillation. Both scenarios show sufficient response times when the feed changes, and the only significant difference between the 1a and 1b is that the COP of the latter is two times higher. It is clear that the “full” MVR integration (2b scenario) offers the largest energy savings among all scenarios, reducing the total specific energy requirements by 76% compared to simple distillation. Compared to “partial” MVR (1b), 2b lowers the external heat requirements by 89%, and thus achieving 58% lower specific energy requirements. This is despite the COP of the heat integration system is reduced by half. Compared to “full” VCHP (2a), it shows half the electricity requirements and 41% lower total specific energy requirements. Despite having 6% of the total heat supplied by an external source, “full” MVR configuration showed high complexity and slow response, and hence, more in-depth optimization of control strategy is required. One the other hand introduction of 3-5% of external heat to “full” VCHP configuration enabled sufficient response and reaching steady state.

Table 3: Overview of the simulation results for all scenarios.

Scenario	COP of the heat integration system	% of total heat demand supplied by the heat integration system	Electricity (kJ/mol)	Total heat (kJ/mol)	Total specific energy (kJ/mol)
Simple distillation	-	-	0	121.8	121.8
Heat pump 1.a	5.2	50.6	11.9	60	71.9
MVR 1.b	10.8	47.18	5.3	64.2	69.5
Heat pump 2.a	2.6	97.2 (100 is possible)	46.1	3.3	49.4
MVR 2.b	5.2	94.12	22.1	7.2	29.3

As discussed, MEG dehydration can be found in several applications where feed and product purities differ. Higher MEG concentrations in bottom product lead to higher temperature difference across the column (including reboiler), and higher MEG concentrations in feed lead to less useable heat in the top vapor. In such cases, “partial” integration scenarios might be promising, as there will not be enough heat for “full” integration and the COP gap (between “partial” and “full”) will be even larger. As explained, “partial” VCHP and MVR scenarios show similar performance, so it is possible that 1a is energetically/economically viable under specific conditions.

Conclusions

The “full” MVR configuration proved to be the most energy efficient, reducing the total specific energy demand of the column by 76% compared to simple distillation and the total steam demand by 94%. It is clearly advantageous over the “full” VCHP configuration that achieved less than half the COP and 59% energy reduction compared to simple distillation. In “partial” integration, the COP of both heat pump systems is doubled, but the total specific energy reduction is limited to a maximum of 43% compared to simple distillation. In contrast with “full” integration , the performance of “partial” integrated MVR and VCHP is comparable, which makes the latter still an option to consider in heat pump assisted distillation concepts. Despite the superior energy performance of “full” MVR concept, “partial” concepts maybe interesting in practice as the intermediate heating at the column is achieved using a falling-film configuration, which also provides other benefits such as debottlenecking and physical footprint reduction.

The control testing showed that a small amount of external heat is necessary to facilitate sufficient response times to feed variations. The current control scheme of the “total” MVR structure is not adequate as steady state could not be achieved after a step change in feed concentration, which was possible in other scenarios. Enhanced control strategies will be investigated in follow-up research as means to improve step-change response of all concepts. Additional work to continue this project will be to simulate the systems for different feed and product purities in order to identify the most promising application and verify the findings in the experimental setting of TNO.

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