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# Energy Saving for Batch Distillation with Mechanical Heat Pumps

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Operational and economic feasibility of different heat-pump systems with mechanical compression integrated to real batch distillation columns are investigated. This study is focused to the reduction of the external energy demand of the batch distillation. The separation of a low relative volatility mixture (n-heptane-toluene) is studied by rigorous simulation performed with a professional dynamic flow-sheet simulator. The distillation column has AE-1000 reactor-reboiler of DIN standard type. The methods studied are vapour recompression, vapour compression and vapour recompression with the application of an external heat exchanger. Operational, heat transfer and economic issues are discussed. We stated that for the VRC in the minimal pay-pack period point the operation time of the batch distillation. For boosting the overall performance of the VC system, we suggested to complete it with an external heat exchanger (VRC-E) where the heat of the compressed top vapour is transferred to the usual heating medium (water). The original VRC system was not economical (payback period much above 10 y). However the payback period of the new VRC-E system was significantly shorter (less than 10 y).

# 1. Introduction

Distillation is one of the most widely used separation methods in the chemical industry in spite of its very high energy demand. The highest heat duties are required by creating the vapour flow in the reboiler (heating) and condensation of the top vapour in the condenser (cooling). The different methods of energy saving which is achieved by means of internal and external heat integrations were widely studied for the continuous distillation process and summarised by Bruinsma and Spoelstra (2010). Kiss et al. (2012) a practical selection scheme of energy efficient distillation technologies is proposed, with a special focus on heat pumps.

The advantages of batch distillation (BD) over the continuous one are well-known. The energy saving methods for batch distillation have been much less studied than for the continuous one. Recently Jana and his co-workers (2011, 2012) investigated the feasibility and efficiency of the vapour recompression system for batch distillation. They proposed the application of variable compression ratio and pointed out the great economical potential of the vapour recompression systems for batch distillation. However they did not study in details the issues of the heat transfer in the reboiler.

The goals of this paper

-to study for batch distillation different heat pump (HP) systems with mechanical vapour compression (vapour recompression with an external heat exchanger),

-the rigorous simulation of the operation (including the heat transfer conditions) of these HP systems integrated to real batch distillation columns,

-to estimate the costs and payback times of these systems and to compare them with those of the conventional batch distillation system.

The calculations are performed with a professional dynamic flow-sheet simulator (CCDCOLUMN, Chemstation, 2007) for the separation of a low relative volatility (n-heptane-toluene) mixture. The reboiler of the systems is of DIN standard types (AE series). For the vapour compression system n-pentane was selected, as working fluid.

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# 2. Heat pump systems with mechanical compression for batch distillation

In a conventional batch distillation column (BD, Figure 1) heat is furnished from the jacket of the reactorreboiler and extracted in the condenser, while the column is considered adiabatic. The reboiler and condenser duties are nearly equal. During the process the temperature of the reboiler ( $T_r$ ) increases, while the temperature of the top vapour ( $T_{top}$ ) increases or it remains nearly constant depending on the operational policy applied (constant reflux ratio (R=const.) or constant distillate composition ( $x_D$ =const.)).





Figure 1: Conventional batch distilation column



Figure 3: Batch distilation column with vapour recompression with external heat exchenger (VRC-E)

Figure 2: Batch distilation column with vapour recompression (VRC)



Figure 4: Batch distilation column with vapour compression (VC)

The objective of a heat pump in distillation is to use the heat of condensation released at the condenser for evaporation in the reboiler. As the temperature in the reboiler is higher a heat pump is required.

By the batch distillation with *vapour recompression* (VRC, Figure 2) the (saturated) top vapour is led to a compressor after it's superheating (protection of the compressor from the liquid break). Then it enters the inner coil (or jacket) of the reactor-reboiler, where it is condensed and the heat is transferred to the reboiler liquid. The condensed liquid is partially refluxed to the top of the column after pressure reduction over a throttle valve. A small trim condenser is needed to balance the heat input, mainly generated by the compressor. The compressor (the heat pump system) is started after the heating-up of the column and works during the production step, only. This flow-sheet is similar to that of Jana and co-workers (2012), but in our case a real reactor-boiler (DIN standards types, AE series) is modelled instead of a theoretical one. The realisation of the batch distillation with vapour recompression raises several issues:

-heating with two different heating media: water steam at the start-up (and eventually during the production as supplementary heating) and organic vapour (mixture) during the production,

-the heating medium contains more than one component therefore the condensation of the top vapour (mixture) happens at variable temperature (between the dew and bubble points),

-the heat transfer coefficient of the condensation of organic vapours is lower than that of water steam,

-the flow rate of the heating medium (top vapour) depends on the heat flow transferred in the reboiler,

-the composition and flow rate of the heating medium (top vapour) usually vary during the production periods (under finite reflux ratio).

In order to eliminate the above drawbacks of the VRC system we propose its modification. In the system vapour recompression with an external heat-exchanger (VRC-E) the compressed top vapour is led to an external heat-exchanger (Figure 3, VRC-E), where the heat is transferred to the usual heating medium (water/steam). That part of water which leaves the heat exchanger still in liquid state is evaporated in an afterheater. In this system there is no need for an inner heating coil in the reboiler and the compressor can be already started when the vapour appears at top of the column.

By the batch distillation with vapour compression (VC, Figure 4) the working fluid is independent of the mixture to be separated. It is evaporated at the condenser, superheated (optional), compressed to a higher (saturation) temperature, condensed in the reboiler and cooled down by expansion over a throttle valve to a (saturation) temperature below the condenser temperature. In this system –similarly to the VRC-E- there is no need for an inner heating coil in the reboiler. The compressor (the heat pump system) can work during the whole process.

# 3. Simulation results

The calculations are performed with a professional dynamic flow-sheet simulator (CCDCOLUMN). The economic evaluation of each configuration is conducted in terms of the payback period of investment (PBP) by combining investment costs, depreciation cost and the yearly savings. The investment cost is estimated by the formula of Douglas (1989).

# 3.1 Basic data

The distillation column has AE-1000 reactor-reboiler of DIN standard type. The number of theoretical stages (N) for each case is 50 (excluding the condenser and reboiler). The separation of a mixture n-heptane-toluene is simulated at atmospheric pressure. The pressure drop of the column is 0.1 bar. The amount of the charge is 6.36 kmol (its volume at 20 C is 0.8 m<sup>3</sup>). It contains 50 mole % n-heptane. At the start of the process the column is empty ("dry start-up"). During the heating-up of the column total reflux is applied. At the end of the start-up, the mole fraction of n-heptane in the distillate ( $x_D$ ) increases to 0.9975. During the production the reflux ratio is 12.

#### 3.2 Batch distillation

The heating medium is water steam of 4 bar. First the duration of the start-up (211 min) and the batch operation time (BOT=801 min), the total (heating) energy demand (SQ=1936 MJ) of the whole process and the recovery of n-heptane (93 %) were determined. The evolution of the heat transfer rate and that of temperature in the reboiler are shown in Figures 5a (beginning of the process) and 5b (whole process). The start-up (Step 1) can be divided into four parts. First (Step1a) the cold charge must be warmed up onto its boiling point. At the beginning the heat transfer rate is high, because the temperature difference between the reactor and heating medium is great. The reactor temperature increases while the heat transfer rate decreases since the temperature difference gets smaller. In the next (Step1b) the liquid starts to boil, suddenly the heat transfer rate jumps up due to the beginning of boiling and then it returns a lower value. After that the column is being filled up with the hold-up (Step 1c), the liquid level in the reboiler decreases) therefore the heat transfer rate slowly decreases. When the column is already filled up with liquid hold-up (Step 1d) the liquid level and the heat transfer rate do not decrease more.



Figure 5: Evolution of the heat transfer rate and temperature in the reboiler

When the distillation column operates already in steady state and the production step (Step 2) starts. (Figure 5b) the reboiler temperature rises more quickly since the more volatile component is withdrawn from the column. The heat transfer rate drops since the heat transfer area reduces (product withdrawal from the column) and the temperature difference diminishes.

It must be still noted that by Jana and his co-workers (2012) the reboiler was heated at a fixed rate.

#### 3.3 Batch distillation with vapour recompression (VRC)

The thermodinamic cycle (pressure (logP)– enthalpy (h) diagram) of the VRC system is shown in Figure 6a.



Figure 6: Thermodynamic cycles for vapour recompression (VRC) and for vapour compression (VC)

The top vapour leaving the column (1: T = 98.52 °C, P = 1.01 bar) enters the process side of the superheater where its temperature is increased by 30 °C in order to prevent the (partial) condensation in the compressor. After then (2: T = 128.52 °C, P = 1.01 bar) it enters the compressor. The compressed (saturated) top vapour (3: T = 161.36 °C, P = 4.55 bar) first condenses (between its dew and bubble point temperatures) and then it cools below its boiling point (4: T = 143.64 °C, P = 4.55 bar) on the utility side of the reboiler. This (subcooled) liquid enters the utility side of the superheater where it cools further (5: T = 120.86 °C, P = 4.55 bar). In the next its pressure and temperature are reduced by a throttle valve (6: T = 98.52 °C, P = 1.01 bar). Finally the vapour-liquid mixture is totally condensed (7: T = 98.52 °C, P = 1.01 bar). One part of the condensate is refluxed to the column, the other part is withdrawn as distillate.

In a VRC system the outlet pressure of the compressor ( $P_{out}$ ) must be at least so high that the bubble point temperature of the top vapour be at least by 15 °C higher than the bubble point of the reboiler liquid (boiling point of the less volatile component at the pressure of the reboiler).

The influence of the outlet pressure on the heat transfer rate, operation time and payback time (Figures 7a and 7b) was investigated. At low values of  $P_{out}$  the heat transfer rate is much lower than in the case of BD when the reboiler is heated with water steam. On the increase of the outlet pressure the heat transfer rate increases therefore the operation time decreases. At  $P_{ou}$  = 4.55 bar the production capacity of the VRC system reaches that of the BD. Figure 7b shows that where the payback period is short enough the

operation time is much longer than that of the BD, that is, there is a considerable decrease of capacity. Where the operation time of the VRC equals to that of the BD, the payback period is near to 15 years, that is, the investment is not economical.



Figure 7: Effect of the compressor outlet pressure on the heat transfer rate (a), on the operation time and payback period (b) in the VRC system

#### 3.4 Batch distillation with vapour recompression with external heat exchanger (VRC-E)

With the application of an external heat exchanger where the compressed top vapour transfers its heat to the usual heating medium (water/steam) the disadvantages of the vapour recompression system can be avoided. However the minimal outlet pressure of the top vapour is higher than for the VRC system since in the VRC-E system its temperature must be at least by 15 °C higher than that of the water steam.

In this system the capacity of the BD can be already ensured at  $P_{out} = .11$  bar and the payback time of the investment is much shorter (8.4 y).

It must be still noted that in the VRC-E system the size of the external heat exchanger has no limit contrary to the VRC where the geometry of the reactor-reboiler limits the heat transfer surface area.

#### 3.5 Batch distillation with vapour compression (VC)

The heat pump can be performed by applying a working fluid which is independent of the mixture to be separated. In this work n-pentane was selected which is widely used as a working fluid (WF). For the inlet and outlet pressures of the compressor the limitations are as follows:

- At P<sub>in</sub> the boiling point of the WF has to be at least by 15 °C lower than the boiling point of the more volatile component at the top pressure. - At P<sub>out</sub> the boiling point of the WF must be at least by 15 °C higher than the boiling point of the less volatile component at the reboiler pressure.

In our case the inlet pressure is at most 4 bar, the outlet pressure is at least 15.7 bar.

The thermodinamic cycle of the VRC system is shown in Figure 6b. The working fluid (1:  $T = 83.03^{\circ}C$ , P = 4 bar) enters the superheater, then (2:  $T = 113.03^{\circ}C$ , P = 4 bar) it is introduced into the compressor. The compressed (saturated) working fluid (3:  $T = 158.77^{\circ}C$ , P = 15.7 bar) first cools to its dew point, condensates and then it cools below its boiling point (4:  $T = 142.71^{\circ}C$ , P = 15.7 bar) on the utility side of the reboiler. This (subcooled) liquid enters the other side of the superheater where it cools further (5:  $T = 123.60^{\circ}C$ , P = 15.7 bar). In the next its pressure and temperature are reduced by a throttle valve (6:  $T = 83.03^{\circ}C$ , P = 4 bar). Finally the vapour-liquid mixture is totally evaporated in the condenser (1).

The influence of the inlet pressure of the compressor ( $P_{in}$ ) on the heat transfer rate in the condenser ( $Q_c$ ), the operation time (Figure 8) and on the payback time (Figure 9) is investigated.

On the decrease of the inlet pressure both the heat transfer rate and the operation time slightly increase whilst the payback time considerably increases. Hence the inlet pressure suggested is 4.0 bar where the payback time is 8.6 y. In the future we intend to study other compounds as working fluid for which the inlet pressure can be atmospheric.



Figure 8: The influence of the inlet pressure on the heat transfer rate in the condenser and the operation time (VC)



Figure 9: The influence of the inlet pressure of the compressor on the payback time (VC)

# 4. Conclusions

Different heat-pump systems with mechanical compression integrated to real batch distillation columns are investigated by focusing to the reduction of the high external energy demand of the process. The separation of a low relative volatility mixture (n-heptane-toluene) is studied by rigorous simulation performed with a professional dynamic flow-sheet simulator. The distillation column has AE-1000 reactorreboiler of DIN standard type. The influence of the most important parameters (e.g. compression ratio) was studied. The heat transfer conditions are investigated and discussed in details. The two basic ways to integrate the heat pump system for a distillation column are the vapour recompression system (VRC), where the working fluid of the heat pump is the top vapour of the column; and the vapour compression system (VC), when the working fluid is independent from the mixture to be separated. In this work for the VC system n-pentane was selected as working fluid. We stated that for the VRC in the minimal pay-pack period point the operation time of the batch process is significantly higher (the production capacity is much lower) than that of the conventional batch distillation. For boosting the overall performance of the VC system, we suggested to complete it with an external heat exchanger (VRC-E) where the heat of the compressed top vapour is transferred to the usual heating medium (water). The original VRC system was not economical (payback period much above 10 y). However the payback period of the new VRC-E system was significantly shorter (less than 10 y).

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