Multidiszciplináris Tudományok, 15. kötet, 4. sz. (2025) pp. 41–47. ***https://doi.org/10.35925/j.multi.2025.4.4***

INVESTIGATION OF ONE-COLUMN AND PRESSURE-SWING DISTILLATION OF ETHANOL-WATER MIXTURE

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Abstract

In this study, the separation of ethanol-water mixture was investigated using the Unisim Design® simulation software with the NRTL activity coefficient model. Two different constructions were investigated: a single high-pressure distillation column (traditional process) and a pressure-swing distillation (PSD) system. It is a relatively difficult separation procedure, because the components make a non-ideal, azeotropic mixture. With the one-column, traditional system the maximum reachable ethanol concentration in the product is equal with the azeotropic value. With the pressure-swing distillation (PSD) system higher ethanol concentration could be achievable in the product, however it has disadvantages (for example the higher costs). During this study the reachable bottom product ethanol concentration is 93 mole%. Some sensitivity analysis was made: the increasing pressure in the second column improves the ethanol mass flow and reduces energy demand in heat exchangers. These results show that pressure-swing distillation is a more efficient alternative technique for ethanol purification over the azeotropic composition in the viewpoint of energy demand in the condensers and reboilers and in the viewpoint of ethanol mass flow in the product.

Keywords: *ethanol-water, heat flow, pressure-swing distillation*

1. Introduction

Distillation is one of the most often used technique in chemical and petrochemical industries to separate from each other the components of liquid mixture. However, it is a very energy-intensive procedure with relatively low thermodynamic efficiency, this is approximately 5-20% (Vane et al., 2010; Javed et al., 2022). In most chemical and petrochemical procedures distillation is approximately 40% of the total operating cost of a plant (Javed et al., 2022; Fang et al., 2019).

Ethanol is an important material in petrochemical processes, it can be used as a solvent or as a raw material or intermediate in chemical synthesis of paints, cosmetics, perfumes, medicine, food etc. (Gil et al., 2008). Furthermore, ethanol is a widespread biofuel, and its utility is growing (Nassif et al., 2022).

Ethanol and water form a non-ideal mixture with azeotropic point. To separate these kinds of components from each other is a very difficult process. There are some alternative techniques which can be used, for instance distillation using salt effects, homogeneous azeotropic distillation, heterogeneous azeotropic distillation and pressure-swing distillation (PSD). This last one is the most economical and in this case two columns operating at different pressures are used (Iqbal and Ahmad, 2016). The

advantage of this method is that this is not require any additional solvent to separate the components from each others (Hegely and Lang, 2021; Battisti et al., 2019).

Due to the azeotropic point is not possible to achieve 100% ethanol product, but with the alternative techniques the ethanol concentration of the product can be increased (Mekala et al., 2022).

Simulation software are powerful tools for design, study and optimize chemical processes. Although, the wrong estimation of physical properties can easily occur inappropriate and inaccurate results. The accuracy of the simulation results based on the thermodynamic model, which should be suitable for the components of the process (Cadoret et al., 2009).

The aim of this study is to investigate and compare the ethanol concentration in the product of a high pressure distillation column and pressure-swing distillation (PSD) system to separate ethanol-water mixture.

2. Simulation and investigation of the distillation

Firstly, in case of investigation of a mixture the vapor-liquid equilibria should be studied (Puentes et al., 2018).

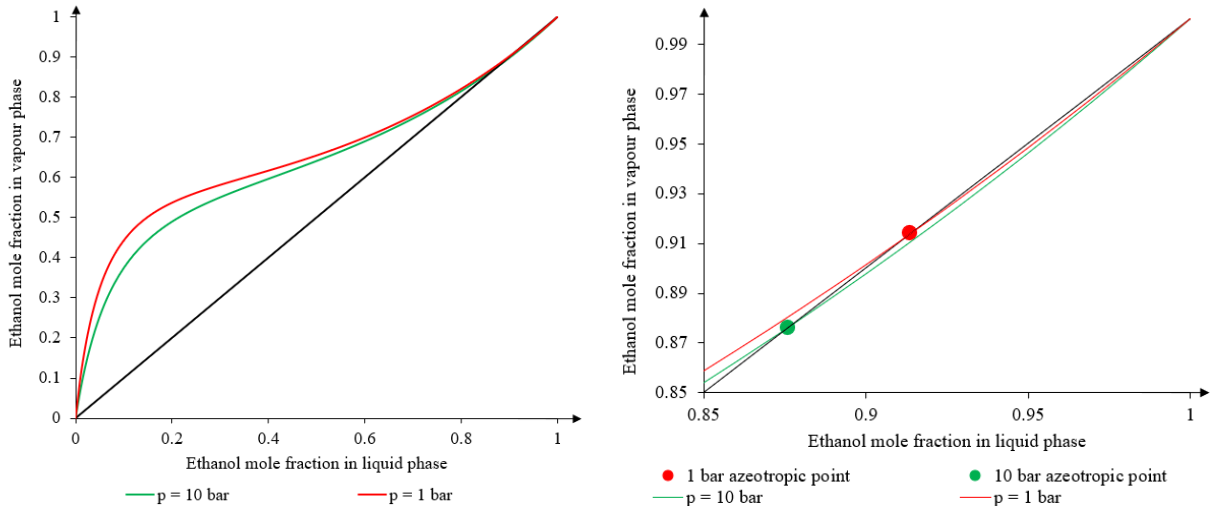

Figure 1. *Equilibrium diagram of ethanol-water mixture at 1 bar$_a$ and 10 bar$_a$ pressure left: the whole equilibrium diagrams, right: detail of the equilibrium curves with the azeotropic points*

Figure 1 shows the equilibrium diagrams of the mixture at 1 bar$_a$ and at 10 bar$_a$ pressures. The diagram demonstrates that the area between the equilibrium curve and the linear is lower with higher pressure and the azeotropic point can be moved. With higher pressure the azeotropic point will be at lower concentration of ethanol. In case of 1 bar$_a$ pressure the azeotropic point is at 0.91 ethanol mole fraction, while in case of 10 bar$_a$ pressure the azeotropic point is at 0.88 ethanol mole fraction. The right part of *Figure 1* demonstrates the azeotropic points. Due to the equilibrium curves are near to the x = y line, the azeotropic point are not so visible.

Pressure-swing distillation system is investigated in the viewpoint of the heat flow of the heat exchangers and mass flow of the product.

The system is studied with Unisim Design® (Unisim Design, 2009) process simulator software with NRTL activity coefficient model (Farajnezhad et al., 2016).

Table 1

Parameters of the feed stream and column

Temperature [°C]	80
Pressure [bar_a]	10
Mass flow [kg/h]	1,000
Ethanol mole fraction	0.5
Water mole fraction	0.5
Reflux ratio	2
Number of theoretical trays	40
Feed tray	32nd*

* The trays are numbered from top to bottom.

In *Table 1* the parameters of the feed stream and main parameters of the column are summarized.

Figure 2 shows the traditional distillation column (traditional means that there are one feed and two products and two heat exchangers in the distillation system) in Unisim Design® environment. *Figure 3* demonstrates also the traditional distillation column, but here the number of trays is marked.

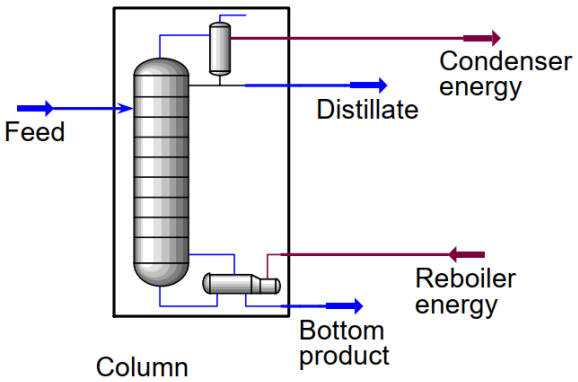

Figure 2. *Traditional distillation system in Unisim Design® environment*

Figure 4 shows the process flow diagram (PFD) of the PSD system and *Figure 5* shows the same in Unisim Design® software environment. There are some differences between the two figures. For example in *Figure 4* there is a so-called Recycle unit operation. It has to use because there is a recycled stream in the system. In *Figure 4* there are boxes around the columns, because software calculates the distillation system as one unit operation with the column, the condenser and the reboiler, as an equilibrium system.

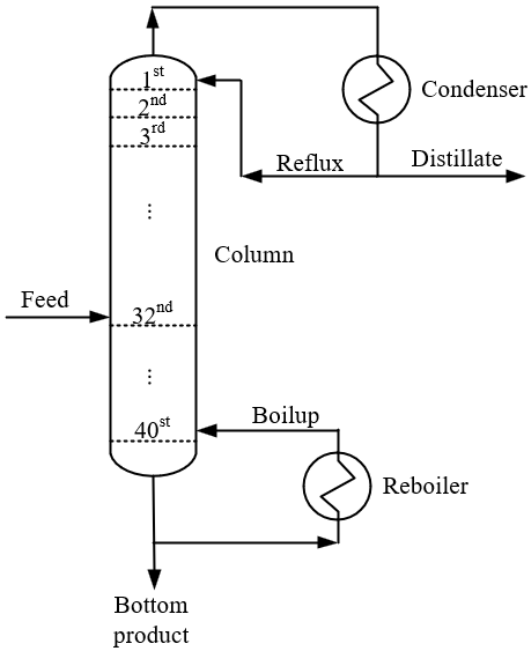

Figure 3. *PFD of the traditional distillation system*

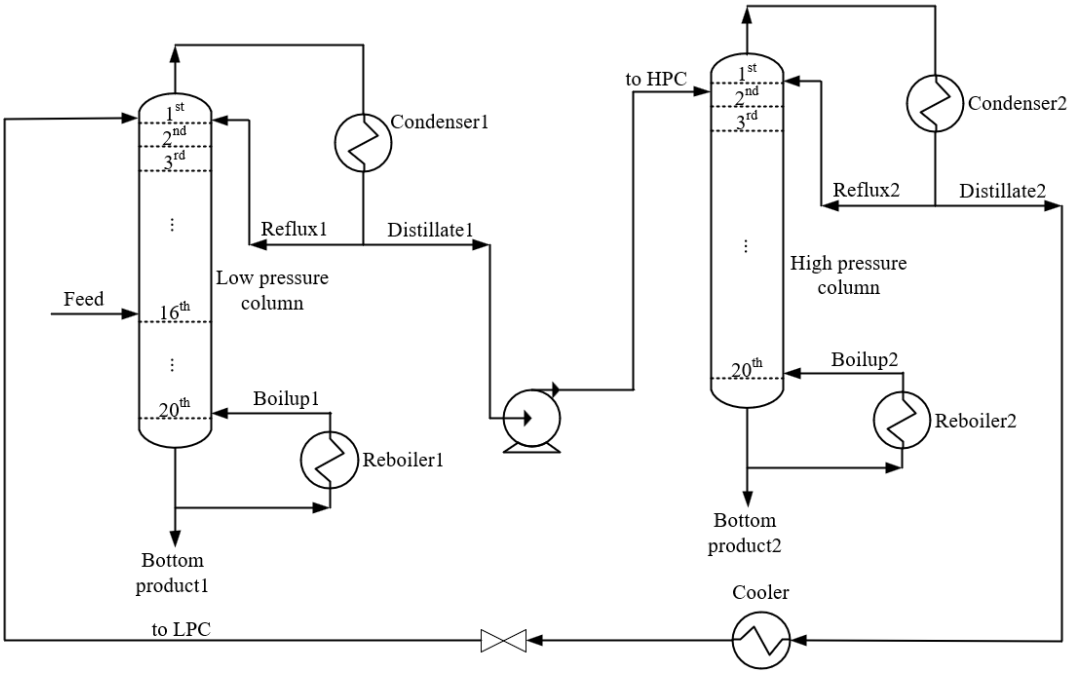

Figure 4. *PFD of the PSD system*

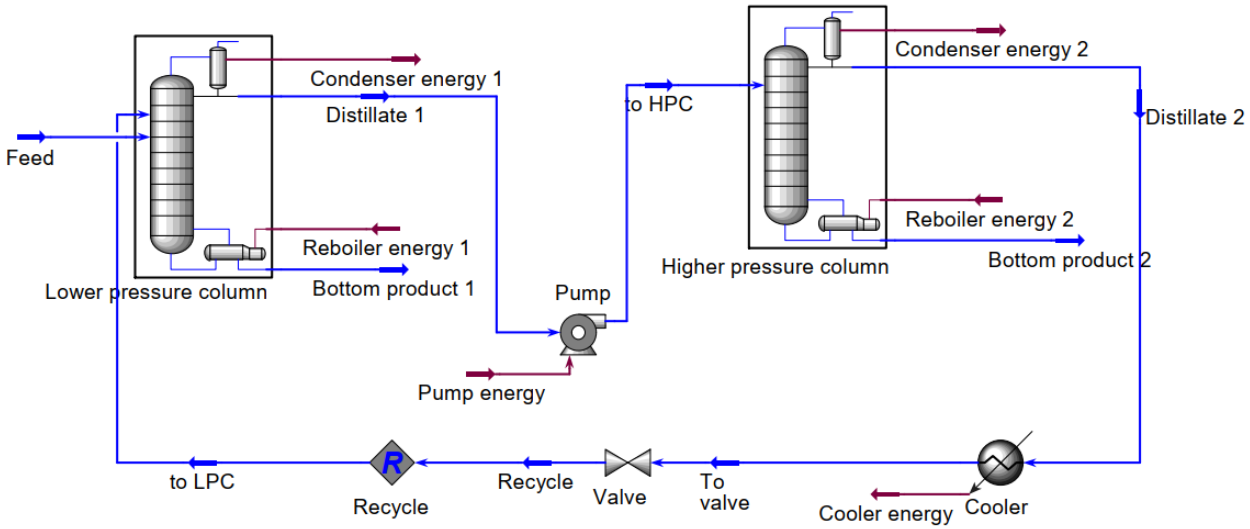

Figure 5. *PFD of the PSD system in Unisim Design® environment*

The first column (Lower pressure column) operates at 1 bar_a pressure with 20 theoretical trays, from these the 16th is the feed tray. The trays are numbered from top to down. The column has another feed from the second column, from that the overhead product is recycled. The reflux ratio is 4. The bottom product of the first column contains 0.999 mole fraction of water. Its overhead product is fed to the second column through a pump, because of the higher pressure.

The second column is operated at 10 bar pressure with 20 theoretical trays and the 2nd one is the feed tray, the trays are numbered from top to down. Its overhead product is recycled to the first column through a cooler and a valve. In the figure there is a Recycle-named virtual object which makes the recirculation possible in the software. The reflux ratio is 0.5. The bottom product2 contains 0.93 mole fraction of ethanol.

The pressures of the columns were chosen by literature, Battisti et al. investigated ethanol-water system to optimize the pressure-swing distillation design in the viewpoint of TAC (Battisti et al., 2019).

2.1. Modification of the pressure in the second column

The pressure of the second column is modified between 10 bar_a and 20 bar_a pressure with 1 bar step size. During the simulations the heat flow of heat exchangers (two condensers and two reboilers) and the mass flow of the Bottom product 2 are studied.

Figure 6 shows the relationship between the pressure of the second column and the heat flow of the heat exchangers. In the figure there three curves are seen, however four heat exchanger data (Condenser1, Reboiler1, Condenser2 and Reboiler2) are demonstrated, the reason for this that the heat flows of the Condenser1 and Reboiler1 are nearly the same. Higher pressure causes lower heat flow in the heat exchangers: twice the pressure means approximately half of the energy requirement.

Figure 7 shows the relationship between the pressure of the second column and the mass flow of the product. Higher pressure causes higher mass flow of the product. It can be seen that the mass flow of the Bottom product2 increases better between 15 and 10 bar than between 15 and 20 bar.

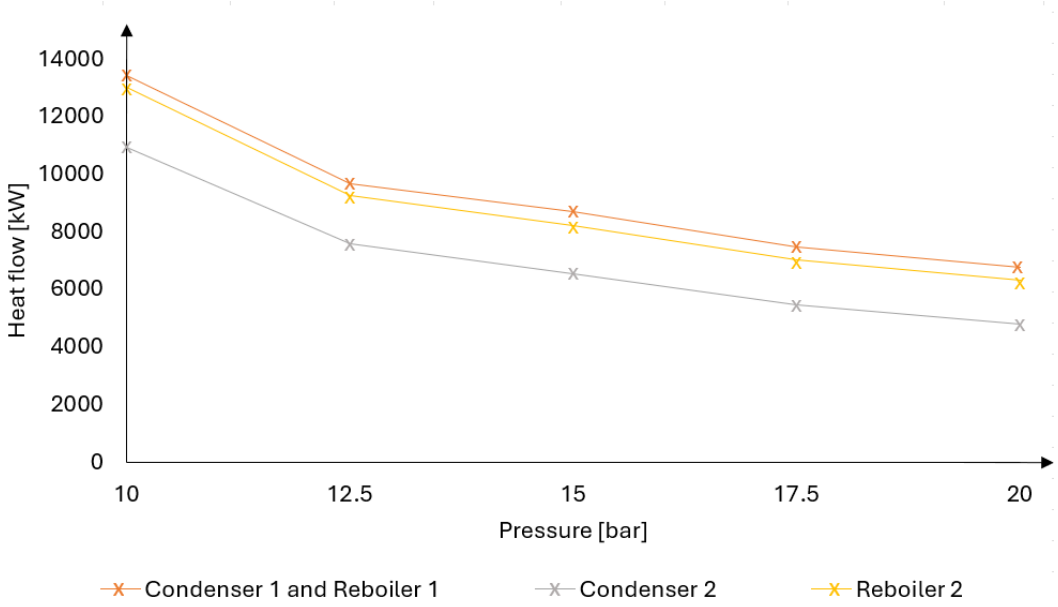

Figure 6. *Relationship between the second column's pressure and heat flow of the heat exchangers*

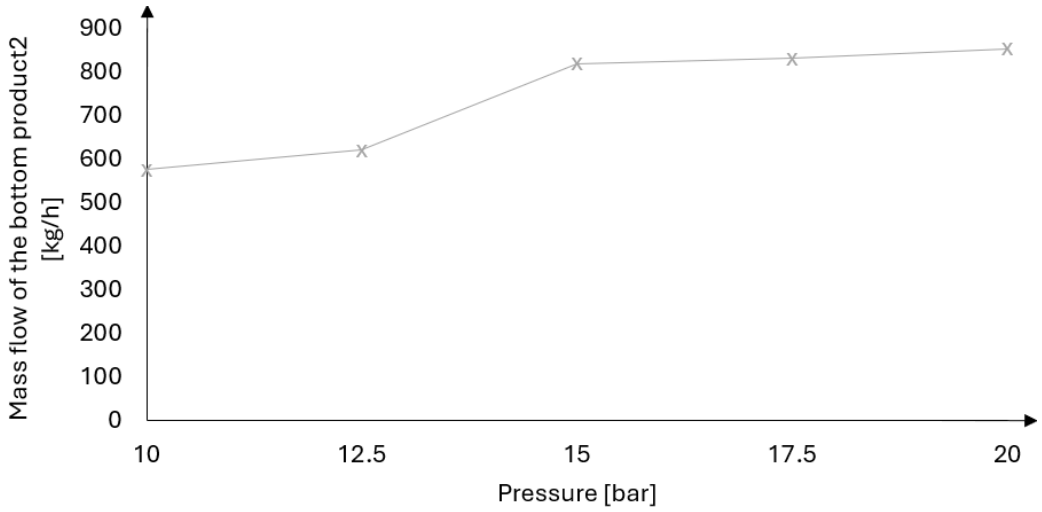

Figure 7. *Relationship between the second column's pressure and mass flow of the product*

3. Summary

During this study distillation of ethanol – water mixture was investigated in the viewpoint of ethanol concentration in the product. Because of the azeotropic point the traditional distillation column is not appropriate to reach more than 88 mole% concentration of ethanol in the product.

It can be concluded that the pressure-swing distillation construction, so with higher pressure in the second column is better in the viewpoint of ethanol mass flow and heat flow of the heat exchangers. However, this system has disadvantages too, for example the higher material and operation costs due to

the higher pressure. In the future the goal is to make a more complex analysis for the PSD system in order to conclude the optimal parameter of the process.

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