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SENSITIVITY ANALYSIS OF HEAT FLOW OF HEAT EXCHANGERS IN ETHANOL-WATER DISTILLATION COLUMN

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Abstract

In this study sensitivity analysis was made with Unisim Design process simulator software for ethanol-water mixture. The effect of the reflux ratio and the number of trays on the heat flow of the heat exchangers was investigated in case of different purification of bottom product. The results of the sensitivity analysis showed that the heat flow of the reboiler averagely 1.94 times higher than the heat flow of the condenser. Afterwards, the effect of the thermal state of the feed stream was investigated on the heat flow of the condenser and the reboiler.

In each cases the mass flow and ethanol content of the distillate stream were also investigated. The results showed that in the studied cases the liquid volume percent of the ethanol varies between 65% and 87%.

A simplified cost estimation was calculated with the determination of mass flow of cooling water and low-pressure steam. From the results it was concluded that higher number of trays, higher temperature of the feed stream and higher ethanol content in the bottom product resulted lower costs of the utility streams.

Keywords: *condenser, reboiler, heat flow, process simulation, distillation*

1. Introduction

Distillation is a widespread procedure in chemical and petrochemical industries, it is primarily used for fluid separation and purification. However, conventional distillation is an energy-intensive technique, and it has a relatively low (approximately 5-20%) thermodynamic efficiency (Javed et al., 2022).

In most chemical and petrochemical processes distillation makes up approximately 40% of the total operating cost of a plant (Javed et al., 2022; Fang et al., 2019). Unfortunately, alternative methods instead of distillation technique, such as molecules separation in according to their size, are expensive to scale up or underdeveloped yet (Sholl and Lively, 2016).

In this study sensitivity analysis was made with Unisim Design (Unisim Design User Guide, 2009) process simulator software, with NRTL (non-random two liquid) activity coefficient model, which is recommended for low pressures (less than 1,000 kPa) and for hydro-alcoholic solutions (Puentes et al., 2018). The usage of activity coefficient models is sometimes difficult or inappropriate because some experimental data is missing or the binary interaction parameters have to be estimated (Cadoret et al., 2009). The vapor-liquid equilibrium of the ethanol-water mixture is relatively well-investigated, thus in the database of simulation software, the necessary parameters are given.

Nowadays, simulation software are powerful tools for design and investigate 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 appropriate thermodynamic model, which is suitable for the components of the process (Cadoret et al., 2009).

2. The investigated systems

The knowledge of vapor-liquid equilibria is the first step of the simulation and optimization of distillation (Puentes et al., 2018). In *Figure 1* the equilibrium diagram of the ethanol-water system is demonstrated, the left one shows the curves between 0 and 1 mole fraction values, while the right one shows the curves between 0.9 and 1 mole fraction values. The mixture has an azeotropic point at the ethanol content of 0.91 mol fraction at the investigated pressure which is one bar$_a$. The azeotropic point is more visible on the right figure.

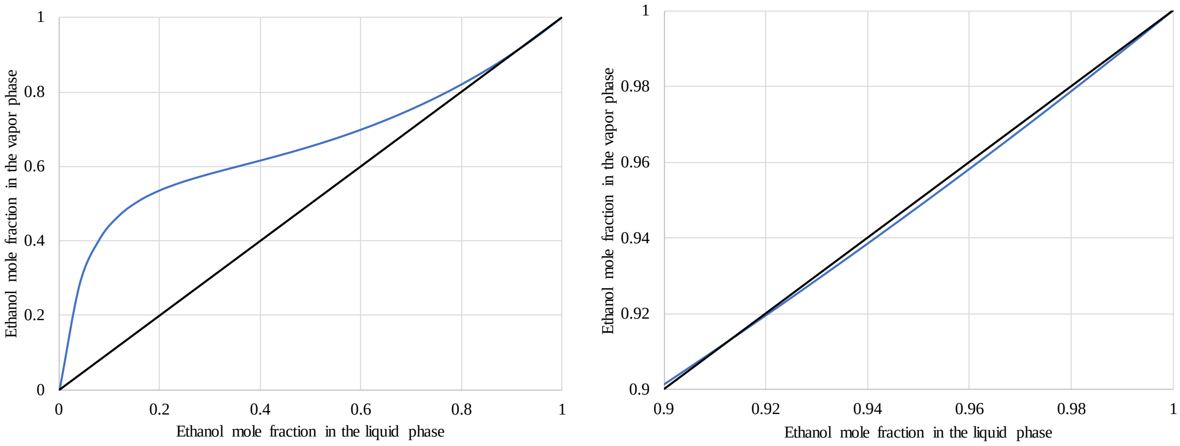

Figure 1. *Total equilibrium diagram of ethanol-water system and the detail of it between 0.9 and 1 mole fraction*

In this study the heat flow of the condenser and reboiler were investigated with sensitivity analysis. The heat exchangers are important part of chemical industry and in the distillation procedure too (Petrik, 2022), and these contribute also to the high costs, so it is necessary to find optimal construction in an operating system with a few modifications of some parameters, like reflux ratio, thermal condition of the feed stream.

2.1. Modification of reflux ratio and the ethanol content of the bottom product

The parameters of the feed of the ethanol-water column are summarized in *Table 1*. Two structures of the column were investigated. In the first case there were 3 theoretical trays in the tower and the second one was the feed tray.

In the other case the number of theoretical trays was 5, and the feed tray was the third one. In these two cases the parameters of the feed were the same and the heat flow of the heat exchangers were investigated if the reflux ratio and the ethanol's liquid volume percent of the bottom product are modified. During the sensitivity analysis the value of the reflux ratio was 0.5, 1, 1.5 and 2. While, the value of the ethanol's liquid volume percent in the bottom product was 1 *V/V*%, 2 *V/V*%, 3 *V/V*%, 4 *V/V*% and 5 *V/V*%.

Table 1. *The parameters of the feed and the products of the ethanol-water rectification column*

Temperature [°C]	20
Pressure [bar$_a$]	1
Thermal condition [–]	cold liquid
Mass flow [kg/h]	5000
Ethanol [V/V%]	15
Water [V/V%]	85

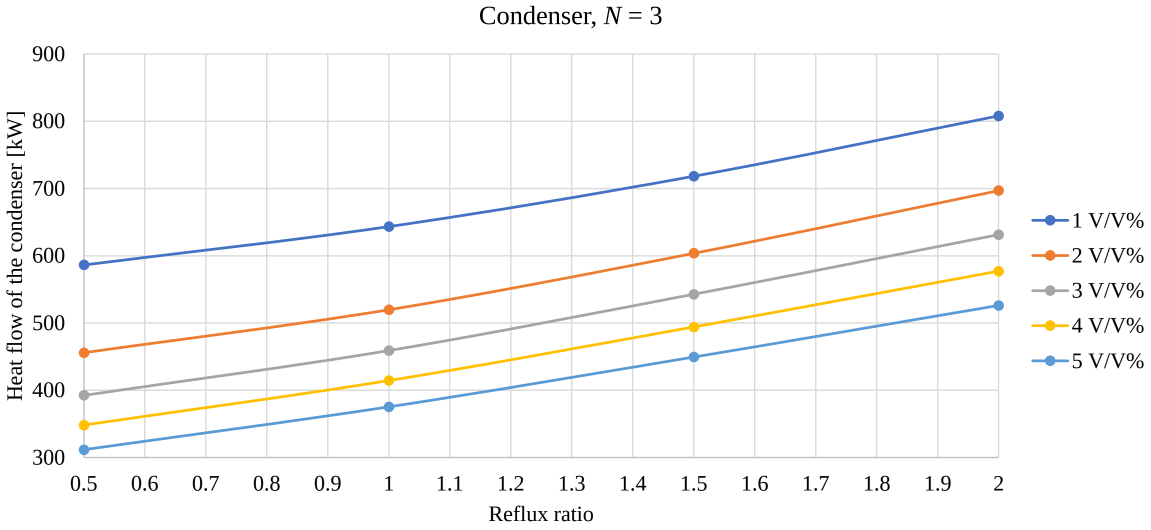

Figure 2. *Heat flow of the condenser in case of different reflux ratio in a three-trayed column*

In *Figure 2* and in *Figure 3* the heat flow of the condenser is demonstrated in the investigated cases. From the results it is determined that higher number of trays in the column (*N*) resulted in lower heat flow in the condenser. Furthermore, it is also concluded that in case of lower ethanol content in the bottom product and higher reflux ratio the heat flow of the condenser is higher.

In *Figure 4* and in *Figure 5* the heat flow of the reboiler is demonstrated in the investigated different cases. From the results it is determined that higher number of theoretical trays in the column *(N)*, higher ethanol content in the bottom product and lower reflux ratio resulted in lower heat flow in the reboiler.

The higher the ethanol content in the bottom product, the lower the differences between the results of the investigated cases. From the results it is also seem, that the heat flow of the reboiler is averagely

1.86 times higher in the three-trayed cases, while averagely 2.03 times higher in the five-trayed cases than the heat flow of the condenser.

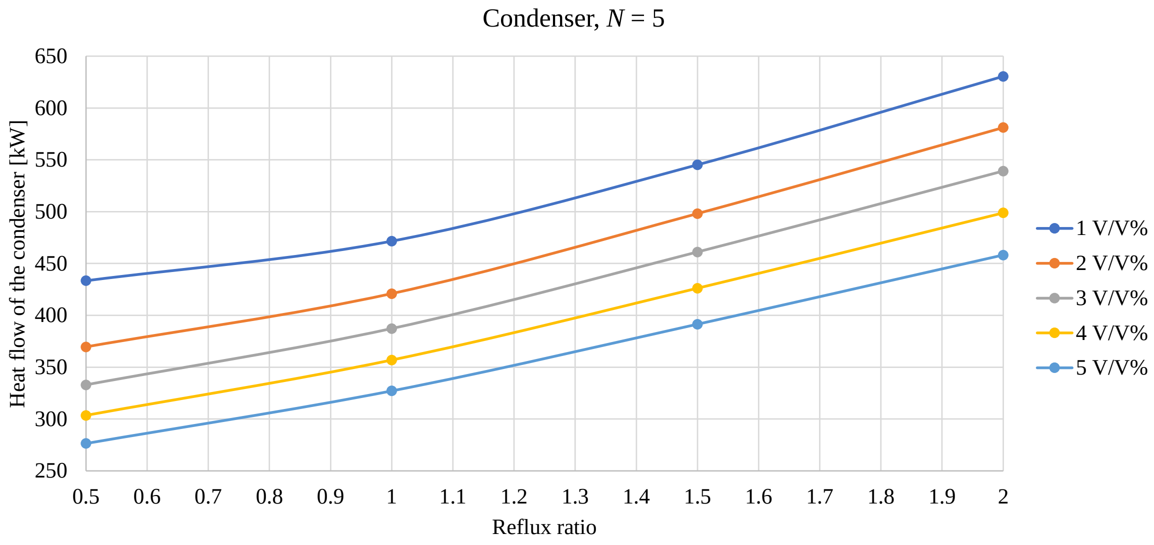

Figure 3. *Heat flow of the condenser in case of different reflux ratio in a five-trayed column*

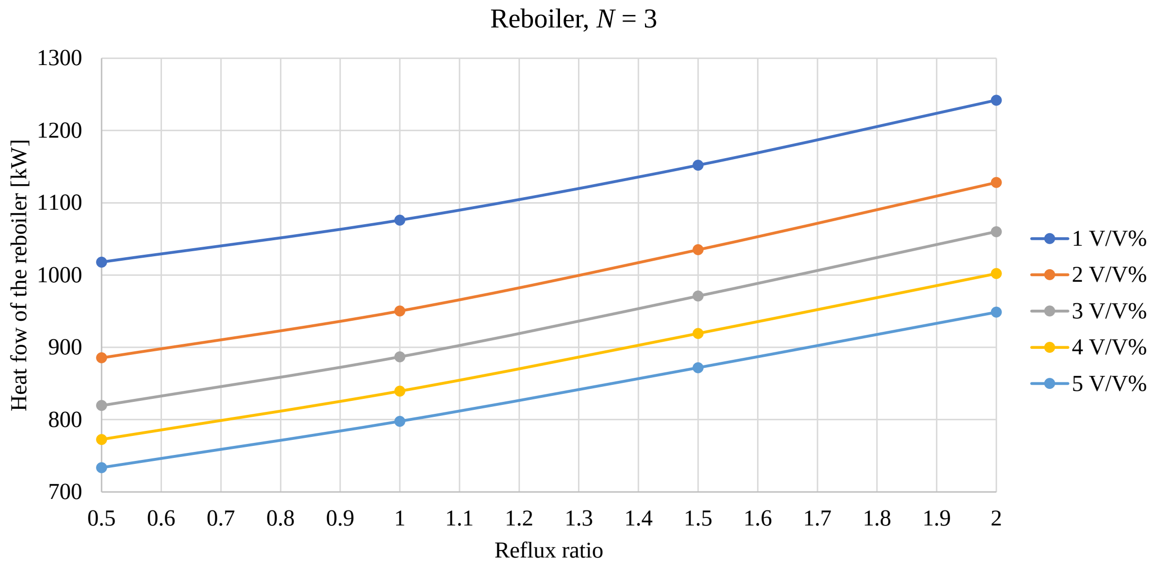

Figure 4. *Heat flow of the reboiler in case of different reflux ratio in a three-trayed column*

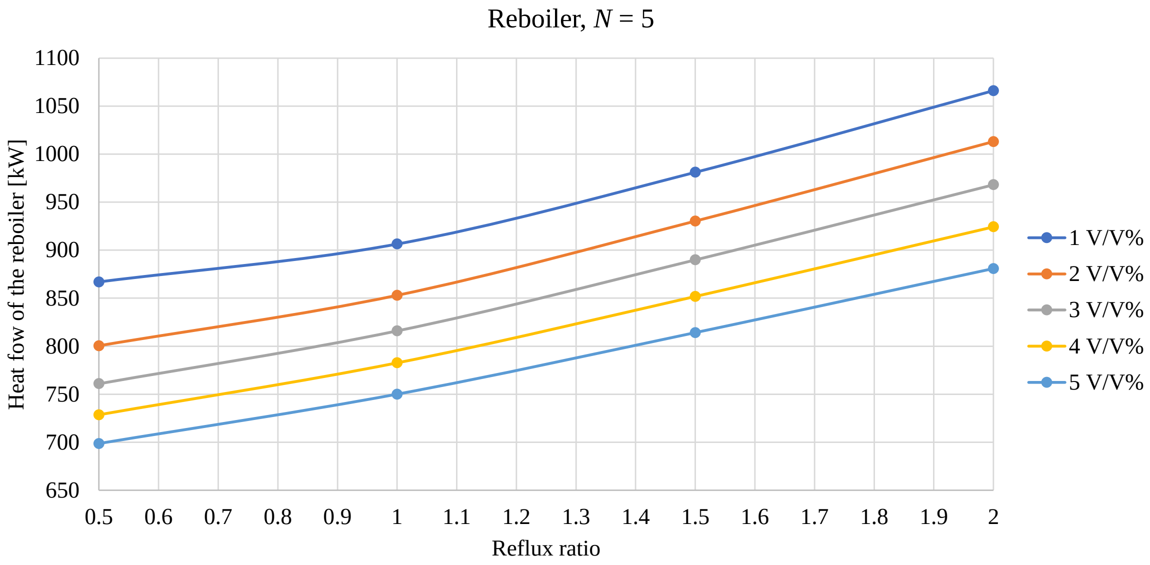

Figure 5. *Heat flow of the reboiler in case of different reflux ratio in a five-trayed column*

In *Table 2* and in *Table 3* the composition and mass flow of the feed stream are summarized in case of different reflux ratio and ethanol content in the bottom product in the three- and five-trayed column. From the results, it is determined that higher ethanol content in the bottom product and higher reflux ratio caused higher ethanol content in the feed product and lower mass flow of the feed stream.

In case of higher number of trays, the ethanol content of the distillate is also higher. As the reflux ratio and the ethanol content in the bottom product increase, the differences between the values of the investigated cases decrease.

Table 2. *The composition and mass flow of the distillate stream in the three-trayed column*

Ethanol content in the bottom product [V/V%]	**R = 0.5**		**R = 1**		**R = 1.5**		**R = 2**	
	x_D [V/V %]	**m_{dist} [kg/h]**	**x_D [V/V %]**	**m_{dist} [kg/h]**	**x_D [V/V %]**	**m_{dist} [kg/h]**	**x_D [V/V %]**	**m_{dist} [kg/h]**
1	65.08	978	71.82	871	75.72	818	77.94	790
2	71.72	822	77.08	754	79.56	725	80.87	711
3	74.61	734	79.01	684	80.88	664	81.91	654
4	76.18	664	79.97	626	81.54	611	82.44	602
5	77.16	603	80.52	571	81.94	559	82.76	552

Table 3. *The composition and mass flow of the distillate stream in the five-trayed column*

Ethanol content in the bottom product [*V/V*%]	**R = 0.5**		**R = 1**		**R = 1.5**		**R = 2**	
	x_D **[*V/V* %]**	m_{dist} **[kg/h]**	x_D **[*V/V* %]**	m_{dist} **[kg/h]**	x_D **[*V/V* %]**	m_{dist} **[kg/h]**	x_D **[*V/V* %]**	m_{dist} **[kg/h]**
1	75.54	820	82.43	739	85.05	711	86.27	699
2	78.91	732	84.16	677	85.98	659	86.90	651
3	80.16	672	84.68	628	86.28	613	87.11	606
4	80.76	618	84.92	581	86.41	568	87.21	561
5	81.17	566	85.04	533	86.47	522	87.26	516

2.2. Modification of the thermal condition of the feed stream

Thereafter, the effect of thermal state of the feed stream on the heat flow of heat exchangers was investigated. Simulations were made with three different thermal states of the feed: cold liquid (T = 20 °C), pre-warmed liquid (T = 55 °C) and liquid at bubble point temperature (T = 89.9 °C).

In *Table 4* and in *Table 5* the results of the condenser's and reboiler's heat flow are summarized in case of three and five number of theoretical trays, in case of the different thermal states of the feed when the reflux ratio is 0.5. The results showed that higher temperature of the feed stream caused lower heat flow in the reboiler, and higher heat flow in the condenser.

In *Table 6* and in *Table 7* the liquid volume percent of the ethanol in the distillate and mass flow of the distillate are summarized. The higher the temperature of the feed, the higher the quantity of the distillate and lower the ethanol content of the distillate. In the viewpoint of the quality of the distillate the lowest temperature of the feed stream is the most appropriate.

Table 4. *The heat flow of the heat exchangers in the three-trayed column*

Ethanol content in the bottom product [*V/V*%]	**Cold liquid (T = 20 °C)**		**Re-warmed liquid (T = 55 °C)**		**Liquid at bubble point temperature (T = 89.9 °C)**	
	$Q_{condenser}$ **[kW]**	$Q_{reboiler}$ **[kW]**	$Q_{condenser}$ **[kW]**	$Q_{reboiler}$ **[kW]**	$Q_{condenser}$ **[kW]**	$Q_{reboiler}$ **[kW]**
1	586.4	1018	643.3	873.4	714.1	743.5
2	455.8	885.5	501.8	730.7	563.5	591.9
3	392.4	819.5	430.3	656.9	485.1	511.3
4	348.1	772.6	380.3	604.3	429.6	453.4
5	311.6	733.5	339.7	561.1	383.9	405.2

Table 5. *The heat flow of the heat exchangers in the five-trayed column*

Ethanol content in the bottom product [*V/V*%]	**Cold liquid (T = 20 °C)**		**Re-warmed liquid (T = 55 °C)**		**Liquid at bubble point temperature (T = 89.9 °C)**	
	$Q_{condenser}$ **[kW]**	$Q_{reboiler}$ **[kW]**	$Q_{condenser}$ **[kW]**	$Q_{reboiler}$ **[kW]**	$Q_{condenser}$ **[kW]**	$Q_{reboiler}$ **[kW]**
1	433.4	866.9	491.1	723.7	569.2	601
2	369.5	800.4	414.6	644.9	482	511.6
3	332.9	761	370.6	598	430.6	457.7
4	303.4	728.5	335.9	560.5	390.3	414.6
5	276.4	698.6	304.9	526.7	354.3	376

Table 6. *The parameters of the distillate in the three-trayed column*

Ethanol content in the bottom product [*V/V*%]	**Cold liquid (T = 20 °C)**		**Re-warmed liquid (T = 55 °C)**		**Liquid at bubble point temperature (T = 89.9 °C)**	
	x_D **[*V/V* %]**	m_{dist} **[kg/h]**	x_D **[*V/V* %]**	m_{dist} **[kg/h]**	x_D **[*V/V* %]**	m_{dist} **[kg/h]**
1	65.08	978	61.88	1037	58.34	1110
2	71.72	822	68.42	870	64.44	934
3	74.61	734	71.44	773	67.34	831
4	76.18	664	73.17	698	69.05	750
5	77.16	603	74.27	632	70.15	679

Table 7. *The parameters of the distillate in the five-trayed column*

Ethanol content in the bottom product [*V/V*%]	**Cold liquid (T = 20 °C)**		**Re-warmed liquid (T = 55 °C)**		**Liquid at bubble point temperature (T = 89.9 °C)**	
	x_D **[*V/V* %]**	m_{dist} **[kg/h]**	x_D **[*V/V* %]**	m_{dist} **[kg/h]**	x_D **[*V/V* %]**	m_{dist} **[kg/h]**
1	75.54	820	71.21	880	66.11	961
2	78.91	732	74.98	779	69.81	849
3	80.16	672	76.54	711	71.42	774
4	80.76	618	77.38	652	72.31	709
5	81.17	566	77.9	596	72.85	648

For the better comparison the negative and positive effect of the thermal state of the feed an easy cost analysis was made. The cost of the necessary quantities of the cooling water and the low pressure (LP) steam were calculated based on the data from (Turton et al., 2009) literature. The necessary quantity of the cooling water (cw) was calculated with the *Equation (1)*, where m_{cw} is the mass flow of the cooling water [kg/h], $Q_{condenser}$ is the heat flow of the condenser [kW], ΔT is the difference between the temperature of the cooling water in the inlet and outlet point [K], c is the average value of the mass heat capacity [kJ/(kgK)].

$$m_{cw} = \frac{Q_{condenser}}{\Delta T \cdot c} \tag{1}$$

In the investigated cases the ΔT was 10 K (because the temperature in the inlet point was 303.15 K, while in the outlet point it was 313.15 K) (Turton et al., 2009), the c was 4.2255 kJ/(kgK).

The necessary quantity of the LP steam was calculated with the *Equation (2)*, where m_{LP} is the mass flow of the LP steam [kg/h], $Q_{reboiler}$ is the heat flow of the reboiler [kW] and r is the mass heat of vaporization [kJ/kg].

In the investigated cases the pressure of the LP steam was 5 bar_g and the vaporization of heat was 2,085.64 kJ/kg.

$$m_{LP} = \frac{Q_{reboiler}}{r} \tag{2}$$

Figure 6 shows the results of the simplified cost estimations of utility streams in case of 3 and 5 number of trays and different ethanol content in the bottom product and different thermal states of the feed stream. The annual cost was calculated with 8,000 hr/year operating hours and according to the literature (Turton et al., 2009) the cost of the LP steam was 29.29 $/1,000 kg and the cost of the cooling water was 14.8 $/1,000 m^3.

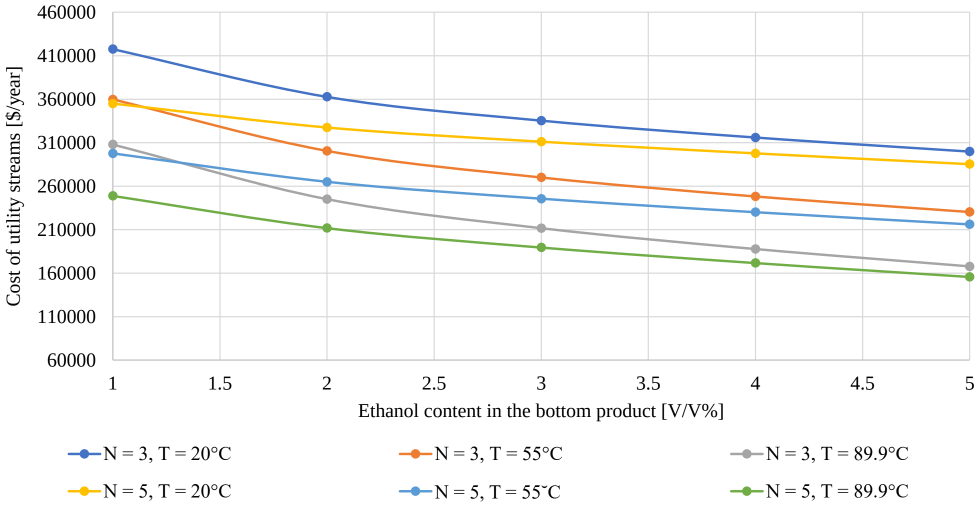

***Figure 6.** Cost of utility streams in the investigated cases*

From the results it is determined that in case of a three-trayed column with cold liquid feed stream has the highest cost of utility streams. However, the five-trayed column with feed stream at bubble point has the lowest cost of utility streams. It is also concluded that the warmer feed results in lower cost of utility streams. In case of the same thermal condition of the feed, the higher the ethanol content in the bottom product the lower the differences between the results of the three- and five-trayed columns.

3. Summary

In this study a widespread known distillation technique, separation of ethanol-water mixture was investigated in the viewpoint of the heat flow of heat exchangers with Unisim Design process simulator software. From the calculated results it is determined that lower reflux ratio and higher ethanol content in the bottom product resulted in lower heat flow in the heat exchangers. The higher number of theoretical trays also resulted in lower heat flow.

With 0.5 reflux ratio and different thermal conditions of the feed stream (cold liquid, pre-warmed liquid and liquid at bubble point temperature) was also investigated the heat flow of the heat exchangers. With literature data a simplified cost estimation was made to determine the costs of the utility streams. From the results it is concluded that higher temperature of the feed stream, higher tray in the column and higher ethanol content in the bottom product resulted in lower costs of the cooling water and the LP steam. Furthermore, in case of the same thermal condition of the feed, the higher the ethanol content in the bottom product the lower the differences between the results of the three- and five-trayed columns.

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