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Ethane-Ethylene Rectification Column's Parametric Examination

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Ethylene is one of the most important product in chemical industry, then it is required to produce ethylene in large quantity. The ethane-ethylene separation is achieved by high pressure cryogenic distillation in a rectification column.

In this paper, an ethane-ethylene rectification column was investigated. At first, the parameters of the column were described, then with two process simulation software – UniSim Design and CHEMCAD –was used to simulate the model of the column.

The purpose of the separation was to reach as much ethylene as possible in the overhead product. Therefore during the parametric examination, the aim was to achieve the greatest – even maximum – quantity and quality of the ethylene in the overhead product. In order to this goal, the influencing effects of the modification of reflux ratio and pressure was evaluated. In addition, changes in the column's internal design (tray construction) was observed. Furthermore, this study examined the behavior of the system (particularly the ethylene mole fraction in the overhead product and the condenser's heat flow) when feed's temperature and mass flow changes.

1. Introduction

Ethylene (C_2H_4) is one of the largest volume petrochemicals produced in world today. The double bond of the ethylene makes it industrially convertible to a variety of intermediate and end products (Benali and Aydin, 2010). Ethane (C_2H_6) is also an important compound in the chemical industry. It is used for producing ethylene or usually in the petrochemicals factories it is recycled in the system, while it is used for heating.

Figure 1 shows that the components do not have azeotrope point, so can be separated from each other in high purification. Nevertheless, as a result of their similar physical behaviour and properties it is difficult to separate them, on the other hand the separation of them is really important. In chemical and petrochemical industries usually these two components are separated with cryogenic high-pressure distillation using in very high rectification column (Liao et al., 2015). Cryogenic distillation is effective, reliable and dominant technology used to separate ethylene from ethane (Shi et al., 2010). However, distillation is still an energy- and capital-intensive process, despite its flexibility and simplicity (Jia et al., 2017).

On the other hand, the lower carbon number molecules – like ethane and ethylene - behave like ideal mixture, as seen in the Figure 1.

In this study an ethane-ethylene rectification column was examined. The goal of the research is to investigate the effects of pressure and reflux ratio to the distillate's compositions. Additionally, the study shows the effects of the different tray types to the column diameter.

Purity and recovery are the most significant design parameters for separation steps and distillation columns can be reliably modelled (Hiller et al., 2015).

Column trays are the most common distillation internals, and these facilitate the contact for gas and liquid. From a point of view of the performance and separation efficiency geometry of the tray is really determinant (Zhao et al., 2018). There are three types of cross-flow trays: sieve, valve and bubble cap. Among them, sieve trays have high capacity and efficiency, low capital cost, but low turndown ratio. Valve and bubble cap trays have also high efficiency, but these have more complicated design than sieve trays (Chuang and Nandakumar, 2000).

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The cost of a tray column is instead of two main factors: column diameter and column height (Chuang and Nandakumar, 2000).

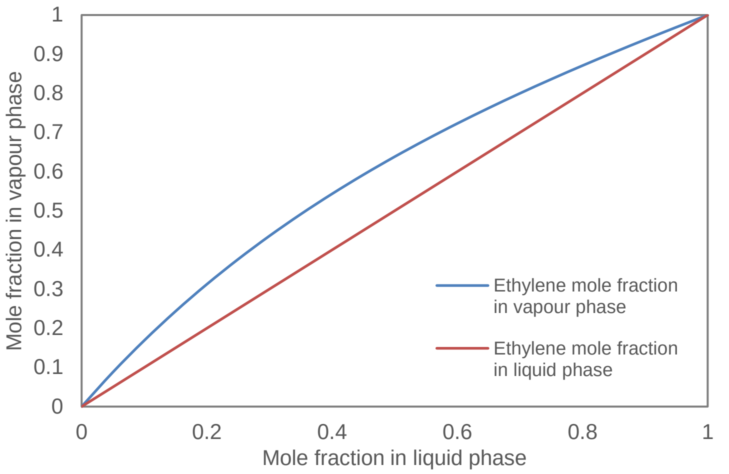

Figure 1: Ethylene and ethane equilibrium diagram

2. Rectification column's technological parameters

The given tower operates with 100 pieces sieve trays, the tray spacing is 400 mm. The feed enters to the 25th stage in vapour fraction to the column, when trays have numbered from bottom to up with the below parameters in the Table 1.

Table 1: Feed parameters

FEED	
Temperature (°C)	-55
Pressure (bar)	7.95
Mass flow (kg/h)	53,750
Composition (%)	
Ethylene	83.3
Ethane	16.7

The restrictions of the separation process are: the ethylene concentration must be 99.95 mol% at the overhead product and the bottom product flow rate must be maximum 10,000 kg/h. The reflux ratio should be 2.2.

2.1. Simulation software

Simulations were prepared with two simulation software, names are UniSim Design (UniSim® Design User Guide, 2009) and CHEMCAD (CHEMCAD User Guide, 2007) process simulator software with SRK model (Jaubert and Privat, 2010). The results were compared with technological parameters (Table 2), these were similar, so modifying in simulations should occur the same alteration in the real system.

Table 2: Products parameters

DISTILLATE	Technological parameters	UniSim Design	CHEMCAD	BOTTOM PRODUCT	Technological parameters	UniSim Design	CHEMCAD
Temperature (°C)	-60.6	-60.49	-60.35	Temperature (°C)	-34.8	-43.08	-42.95
Pressure (bar)	7.48	7.45	7.45	Pressure (bar)	7.48	7.45	7.45
Mass flow (kg/h)	44,200	44,266	43,777.26	Mass flow (kg/h)	9,550	9,484	9,972.7
Composition (%)				Composition (%)			
Ethylene	99.95	99.998	99.997	Ethylene	2.136	5.3	5
Ethane	0.05	0.002	0.003	Ethane	98.864	94.73	94.99

To simulate this system, it is necessary to determine the degrees of freedom of the column. In this case a total condenser was used, so two specifications had to be determined. These were the restrictions of the reflux ratio, the maximum flow rate of the bottom product, or the ethylene mole fraction in the overhead product. Usage of them depended on what parameter was examined.

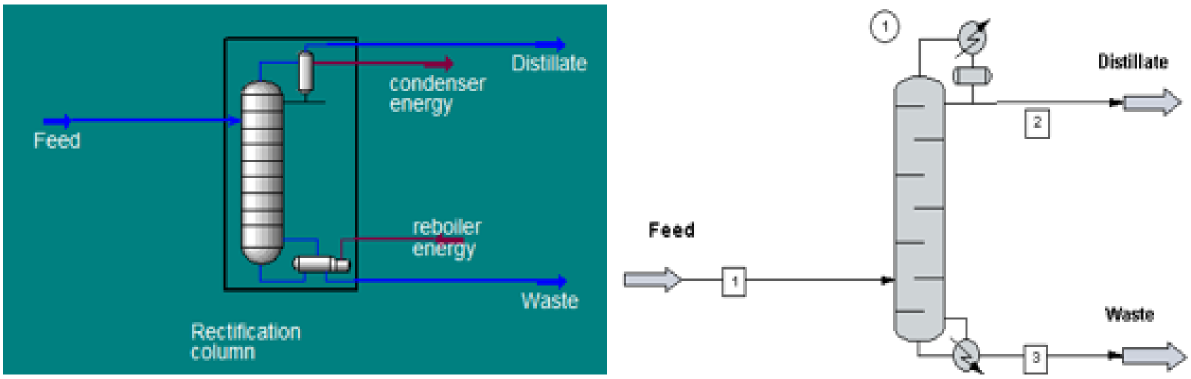

Figure 2: Rectification column's model with UniSim Design and CHEMCAD software

3. Parameter examination

3.1. Modifying pressure

One of the most significant column's parameter is the pressure. As pressure increases, tray column can tolerate the pressure drop across the trays and become more efficient for mass transfer (Chuang and Nandakumar, 2000). Perspective the purification of ethylene and the mass flow of ethylene in the distillate pressure cannot occur numerous changes. With the technological parameters, what are given, to modify pressure in 1 to 10 bar the specification to the purification and mass flow of the distillate can succeed. On the other hand, pressure has the influence to another important parameter, to the heat flow of the reboiler. Therefore, between pressure and temperature there is an obvious connection, decreasing pressure results in higher energy consumption in the reboiler.
Like Figure 3 shows, the suitable pressure value – considering the reboiler's heat flow – is between 8 and 10 bars.

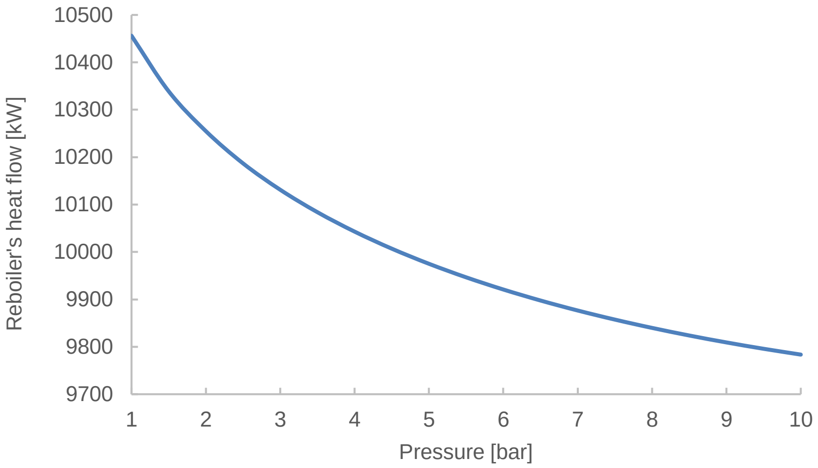

Figure 3: Pressure's influence on reboiler's energy consumption

3.2. Effects of reflux ratio

Reflux ratio is the parameter that can influence mostly the ethylene mole fraction in the distillate. However, effects of reflux ratio are complicated, because if the reflux ratio is low the separation will not be appropriate, even if the reflux ratio is too big column's diameter and heat flow of the condenser will increase. It is necessary to find an optimal solution (Cai et al., 2011).

During the parameter examination the simulation was prepared with reflux ratio values from 1 to 3 with 0.1 interval steps, while the other parameters were kept the same as mentioned in Table 1. The results in Figure 4 show that above 2.3 reflux ratio overhead product contains only ethylene, and between 1.9 and 2.3 reflux ratio values the desired purification can be reached. However, below 1.9 value the mole fraction of ethylene is not enough.

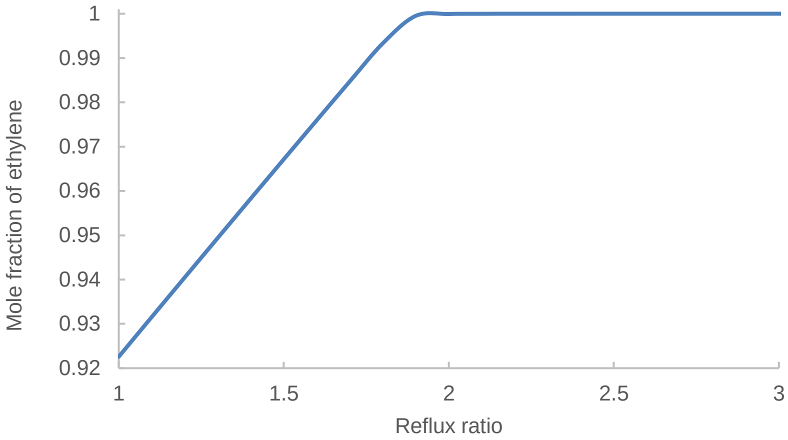

Figure 4: Reflux ratio's influence to the mole fraction of ethylene

3.3. Modification of tray types

The examined column's internal consists of trays. Column's diameter is one of the most determinative parameters in terms of costs. Simulations show that three types of trays can be used for the exercise, these are sieve, valve and bubble cap trays. All three result in the expected purification, but the column's diameter is different in each case.

In Table 3 the calculated and simulated data are summarized. Calculations were done according to Souders-Brown-Fair and F-factor methods (Fonyó and Fábry, 1998).

F-factor method calculations result in the same column diameter in each type, because in the enumeration the determining parameter is the pressure and the tray spacing, these are the same in every case. While in the Souders-Brown-Fair method the determinative parameters are – besides the tray spacing – mass flow and density of vapour and liquid phase.

In the software one of the essential view point of the measurement was the function of flooding, what determines the minimum possible diameter of the column. Because if the flooding velocity is higher than 80 percent, the separation will not have the expected efficiency (Perry at al., 1997).

Table 3: Column diameters (Reflux ratio = 2.2)

Tray type	SBF method (m)	F-factor method (m)	UniSim Design (m)	CHEMCAD (m)
Sieve	4.25	3.22	4.76	5.029
Valve	4.25	3.22	3.2	3.5
Bubble cap	3.89	3.22	4.115	4.115

Like it was mentioned, reflux ratio has the influence on the column diameter. In case of reflux ratio is 1.9 column's diameter decrease, while the overhead product has convenient quality and quantity. Table 4 shows the results of calculations and simulations.

Table 4: Column diameters (Reflux ratio = 1.9)

Tray type	SBF method (m)	F-factor method (m)	UniSim Design (m)	CHEMCAD (m)
Sieve	4.03	3.06	3.658	4.87
Valve	4.03	3.06	3.048	3.35
Bubble cap	3.67	3.06	3.81	3.962

3.4 Modification of feed parameters

In industry malfunction can sometimes occur, due to that, the operation of the tower and the parameters of the feed can be modified. Therefore, this study examined what will happen if the temperature, mass flow of the feed changes and which consequences will be to the condenser's heat flow or to the ethylene composition in the overhead product. Because the temperature defines the vapour fraction of the feed, therefore, changing the temperature, the separation's operation will not be the same.

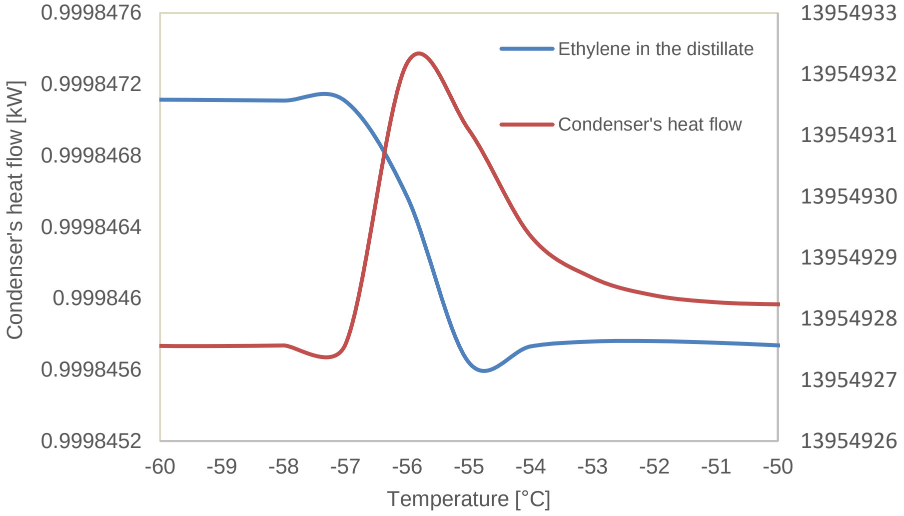

Figure 5: Relationship between the feed's temperature and the condenser's heat flow, as well as the distillate's quality

In case of lower temperature – when the feed is liquid - causes lower heat flow in the condenser, moreover there is higher concentration of ethylene in the overhead product. While the feed temperature is higher, the results are less fortunate from the viewpoint of the operational costs and product purity. In this case according to the Figure 5 the feed temperature change is negligible for the quality of the overhead product in the examined temperature range.

In case of malfunction not only the temperature, but also the mass flow of the feed can change. Table 5 summarizes, what could happen if the mass flow of the feed increased or decreased by 10 % of its technological data.

Table 5: Connection between mass flow of the feed and bottom product

Feed's mass flow (kg/h)	Bottom product's mass flow (kg/h)
53,750	9,484
48,375 (90%)	8,535
59,125 (110%)	10,430

During the simulation the degrees of freedom of the column were the reflux ratio and the restriction of the ethylene composition in the distillate. Table 5 shows, that higher feed's mass flow occurs higher bottom product's mass flow, than the allowed value. But, when the bottom product's mass flow is limited to 10,000kg/h the simulations showed that the ethylene mole fraction in the distillate is only 0.9913 which is lower than expected.

4. Conclusions

Because of the importance of ethylene, it is necessary to produce it in high purity. If high purity product is required it should be the distillate product, however, there are other essential factors, like the optimal energy consumption and economic factors like costs.

The results of the parameter examination show that in the case of the industrial case study the operating pressure is suitable. The reflux ratio is higher than needed causing higher energy consumption and the column diameter should be also higher, the costs will increase too. This study proves that lower reflux ratio is appropriate because this separation also satisfies the requirements. Beside the lower energy consumption, a smaller column diameter proves to be also satisfactory.

To investigate the type of column trays according to the Souders-Brown-Fair method the bubble cap tray column has the least diameter, while the F-factor method results in the same and small diameter values. According to the simulations the valve trays are the most convenient for the problem because with this type of flexible column internal the column has the lowest diameter, so it occurs the lowest investment costs.
Examining the effect of the feed temperature, the results show that it has not significant influence on the product quality and the condenser's energy consumption in the examined temperature region. When quantity of feed is decreased or increased with 10% compared to the operating point, the requested purity of the overhead product is not satisfactory.

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References

Benali M., Aydin B., 2010, Ethane/ethylene and propane/propylene separation in hybrid membrane distillation systems: Optimization and economic analysis, Separation and Purification Technology, 73(3), 377–390.

Cai J., Cui X., Yang Z., 2011, Simulation for transesterification of methyl acetate and n-butanol in a reactive and extractive distillation column using ionic liquids as entrainer and catalyst, Chinese Journal of Chemical Engineering. Chemical Industry and Engineering Society of China (CIESC) and Chemical Industry Press (CIP), 19(5), 754–762.

CHEMCAD User Guide, 2007, CHEMCAD Version 6 User Guidem, <www.coursehero.com/file/16683076/CHEMCAD-6-User-Guide-2012/> accessed 14.6.2018

Chuang K.T., Nandakumar K., 2000, Tray Columns: Design, Distillation - Tray Columns: Design, 1, 1135–1140.

Fonyó Z., Fábry G., 1998, Vegyipari művelettani alapismeretek, Nemzeti Tankönyvkiadó Rt., Budapest, Hungary.

Hiller C., Meier R., Niggemann G., Rix A., 2015, Distillation in special chemistry, Chemical Engineering Research and Design, 99, 220–227.

Jaubert J.N., Privat R., 2010, Relationship between the binary interaction parameters (kij) of the Peng-Robinson and those of the Soave-Redlich-Kwong equations of state: Application to the definition of the PR2SRK model, Fluid Phase Equilibria, 295(1), 26–37.

Jia S., Qian X., Yuan X., 2017, Optimal design for dividing wall column using support vector machine and particle swarm optimization, Chemical Engineering Research and Design, 125, 422–432.

Liao P.Q., Zhang W.X., Zhang J.P., Chen X.M., 2015, Efficient purification of ethene by an ethane-trapping metal-organic framework, Nature Communications, 6, 1–9.

Perry R.H., Green D.W., Maloney J.O., 1997, Perry's Chemical Engineers' Handbook Seventh, McGraw-Hill, New York, USA.

Shi M., Lin C.C.H., Kuznicki T.M., Hashisho Z., Kuznicki S.M., 2010, Separation of a binary mixture of ethylene and ethane by adsorption on Na-ETS-10, Chemical Engineering Science, 65(11), 3494–3498.

UniSim® Design User Guide, 2009, <ftp://tzin.bgu.ac.il/shacham/ProcDes17_18/User%20Guide.pdf> accessed 14.6.2018.

Zhao, H., Li L., Jin J., Li Q., 2018, CFD simulation of sieve-fixed valve tray hydrodynamics, Chemical Engineering Research and Design, 129, 55–63.