INTERNATIONAL JOURNAL ON ORANGE TECHNOLOGY

https://journals.researchparks.org/index.php/IJOT e-ISSN: 2615-8140 | p-ISSN: 2615-7071

Volume: 03 Issue: 11 |Nov 2021

Modeling and Simulation of the Process of Natural Gas Fractionation

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Abstract: In this work, the steady-state model of the process of natural gas fractionation was developed and analyzed using Aspen Plus. Mixture of gases after primary separation was obtained as a selected gas, and this product consists of 68% and 32% of propane and butane, respectively. The optimal reflux ratio and product purity were calculated considering the minimal energy consumption of the reboiler and cooler. The flexibility of the actual column and the change in the number of stages for different types of flowrates were investigated. In addition, optimal feed stage have been found according to overall efficiency for product quality and energy consumption of reboiler and cooler.

Keywords: propane-butane fraction, modeling, optimization, reflux ratio, product purity, efficiency.

Introduction

The method of separation by distillation is an important one for separating natural gas fractions. Despite the fact that there are many gas processing companies in our country, the separation of propane-butane fraction into specific components is not widespread. The propane-butane mixture selected for the modeling process is the product obtained after separation of light fraction from the content of natural gas to propane, and their molar proportion is 0.68 and 0.32, respectively. In this case, a clean propane in distillation column should be separated from the butane and a few other heavy fractions contained in the natural gas.

The purpose of this article is to model the distillation method of the propane-butane mixture in the Aspen Plus program and to observe the effect of the main parameters on the product purity and the amount of energy consumed by the reboiler.

Modeling of processes through computer programs can be considered as a virtual expression of the technological processes via mathematical model, taking into account its physical and chemical properties. Using this method, it is possible to predict, design and optimize data for various situations that may occur in the production process [1].

A process simulator is an instrument that offers the numerical solution of a mathematical model, which includes elements such as:

- Components database, which contains the needed values for the calculation of physical properties starting from the thermodynamic models.
- Thermodynamic models section that offers a wide range of options for the calculation of liquid-vapor (LVE) and liquid-liquid (LLE) equilibriums, enthalpies and other thermodynamic properties.
- Flowsheet section, related with the flows and equipment under analysis.
- Operating units section, for the realization of matter and energy balances in the different units of operation.
- Output Generator section, it returns a whole report of the simulation results.
- Calculus sequence section that controls the calculation sequence and the simulation convergence.

Objects and methods of research.

2.1 Thermodynamic properties

A model or simulation model represented by a computer program incorporates a set of mathematical expressions that indicate the properties of the devices involved. These equations have variable parameters that combine the physical and thermodynamic properties of the components and compounds involved in the process. It is necessary to define the parameters such as temperature, pressure, component

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concentration, and specific values for each component, for the correct selection of these parameters and mathematical expressions. We know that each individual component or compound has its own thermodynamic properties. When designing any model, it requires the physical, chemical and thermodynamic properties of the components and compounds. In order to be closer to the production process, the model needs to be added to all components involved in the process, and all possible conditions (concentration, temperature, pressure, etc.) [2].

The Soave-Redlich-Kwong state equation is chosen as the thermodynamic property model and as indicated in the literature, it can be used for light hydrocarbon gases[3].

This equation is given below:

$$P = \frac{RT}{v_m + c - b} - \frac{a(T)}{(v_m + c)((v_m + c + b)} \quad (1)$$

Here, *T*-temperature, *P*-pressure, v_m-molar volume and *a*, *b*, *c* coefficients are defined as follows:

$$a = \sum\sum x_i x_j a_{ij} + \sum a"_{wi} x_w{}^2 x_i \quad (2)$$

$$b = \sum x_i b_i \quad (3)$$

$$c = \sum x_i c_i \quad (4)$$

Here, *x_i* and *x_j* correspond respectively to the molar fraction of components *i* and *j* in the mixture.

The simulation modeling process does not only require the most advanced software or simulator software from the well-known companies, but also the thermodynamic method appropriate to the selected model, components, and compounds. If the incorrect thermodynamic method is selected during the process of modeling, it is not compatible with the real results of the modeling process, which may not be adequate enough. However, it is not an easy task to determine which thermodynamic approach is acceptable for all compounds or components in the process. One of the ways to choose the best fitting thermodynamic method is to select the range of expected results. The thermodynamic properties of any component depend on the nature of its molecule. Therefore, in order to summarize the properties of the flowsheets involved in the process, it is necessary to be familiar with the nature of all the molecules. Existing theoretical sources for evaluating the properties may also be of a rational type (based on kinetic theory of thermodynamic laws and molecular nature), experimental type (experimental data correlated with mathematical expression), or combination of both. Certainly, empirical correlation methods are an effective one, but when the values are exceeded, these correlation methods may not be adequate to the real process. In general, the reliability of correlation depends on the reliability of theoretical foundations, especially when this correlation is proved by experimental data. If theoretical basis is insufficient, then it is recommended to build a model based on experimental data.

The propane / butane separation columns are schematically represented in Figure 1. **Table 1** introduces the initial parameters that are needed to model this process using computer programs.

Table 1: The initial experimental results for modeling the mixture of propane / butane.

Stream components	Molar proportion, %	Obtaining source
CO_2	3,36	the primary processing of natural gas in Shurtan chemical complex
H_2S	0,06	
CH_4	88,74	
C_2H_6	4,08	
C_3H_8	0,89	
C_4H_{10}	0,41	
C_5 hydrocarbons	0,17	

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C_6 and higher hydrocarbons	0,3	
N_2	0,76	
H_2O	1,23	

According to the data presented in the **Table**, if we assume the propane / butane mixture are separated from the processing of natural gas, then the amount of propane in the mixture consists of 68 of the molar ratio.

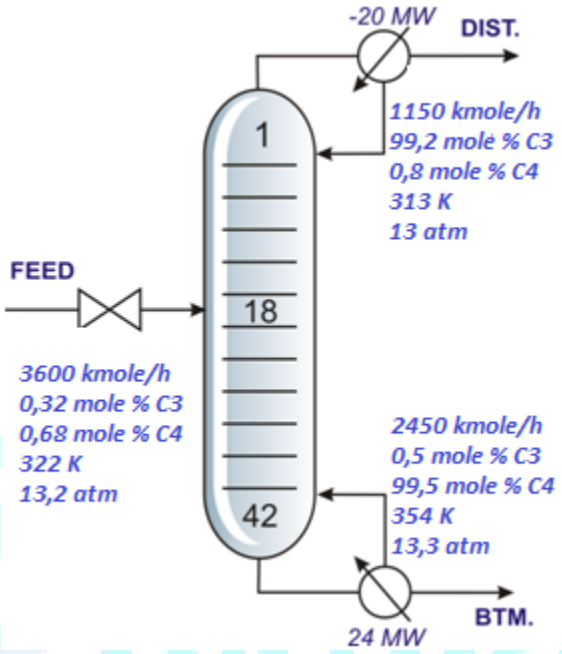

Figure 1. The schematic view of the propane-butane mixture separation column.

The RADFRAC block has been selected in the Aspen Plus program for modeling the rectification column in this study, which is a tool for a thorough investigation of the fractionation process of all types of multistage liquid-vapour phases. Despite the fact that RADFRAC block representing Rectification (Distillation) process is based on state balance models, the Murphree efficiency can be taken into account, in line with the compatibility to real processes in production.

The reflux rate in the column is selected based on the sensitivity analysis, the efficiency of the cooler/reboiler and the product purity, and the number of reflux needed to achieve optimal efficiency is 3.7 mol. [3]

2.2. Propane / butane binary system.

The propane / butane being investigated is 3600 kmol / hour in the binary system, with the molar proportion of butane (32%) as mentioned above. The column pressure is 13 atm (in order to select the water as a cooling agent), where cold water and medium pressure steam can be used for cooling and heating operation (Fig. 2). The minimum amount of cleanliness in the separation of the mixture, in this case, is 99 percent per component, including 42 plates-cooler/reboiler together, plus 14 plates as the starting point for the column (**Table 2**).

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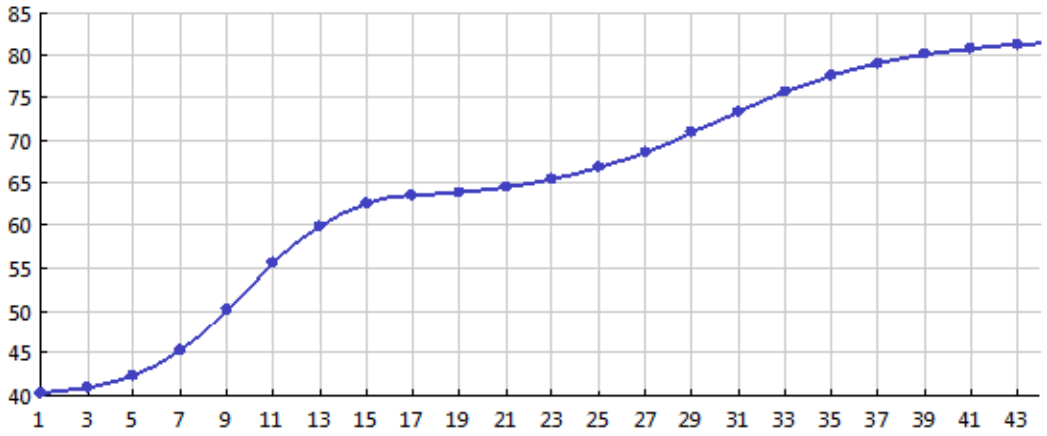

Figure 2.Temperature change in the rectification column. X-axis is the temperature C, Y-axis is the number of plates.

Table 2. The dependence of the separating product purity and the change in energy consumption on the number of plates.

Plates	The number of plates	Purity of bottom stream, weight %	Distillation purity, weight %	Energy consumption of the reboiler, gkal/hour	Energy consumption of the cooler, gkal/hour
1	30	0,9968	0,9576	20,4225	-17,7622
2	31	0,9968	0,9631	20,4073	-17,7367
3	32	0,9968	0,9679	20,3954	-17,7156
4	33	0,9968	0,9720	20,3854	-17,6975
5	34	0,9968	0,9755	20,3772	-17,6819
6	35	0,9968	0,9784	20,3705	-17,6685
7	36	0,9968	0,9809	20,3651	-17,6572
8	37	0,9968	0,9831	20,3610	-17,6477
9	38	0,9968	0,9848	20,3579	-17,6397
10	39	0,9968	0,9863	20,3557	-17,6330
11	40	0,9968	0,9875	20,3543	-17,6275
12	41	0,9968	0,9885	20,3536	-17,6230
13	42	0,9968	0,9930	20,3535	-17,6194
14	43	0,9968	0,9911	20,3538	-17,6165

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2.3. Selection of the feed stage in the column

In order to meet these criteria, when the temperature of the input mixture to column and reflux ratio are constant, the stage (plate) is chosen, in which product purity is the highest. In this case, many of the feed stage of plates can be selected. According to the results of the modeling, the recommended step for the compound we are looking at is the 18th step and through this point distillate and bottom stream are the highest (**Fig.3**).

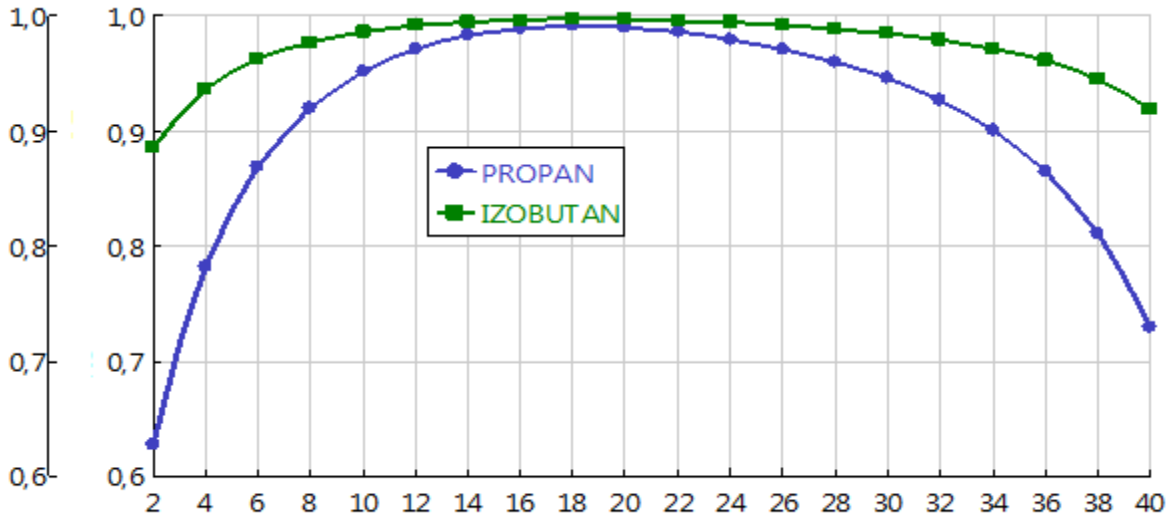

Figure 3. The graph of the dependence of product purity separating propane/butane compounds on the feed stage. X-axes are the purity of the distillate and bottom stream, Y-axis is the number of plates.

In addition, the minimum amount of energy consumed by the reboiler is considered as the main principle when selecting the feed stage, which is based on the sensitivity analysis of the Aspen Plus program (**Fig. 4**).

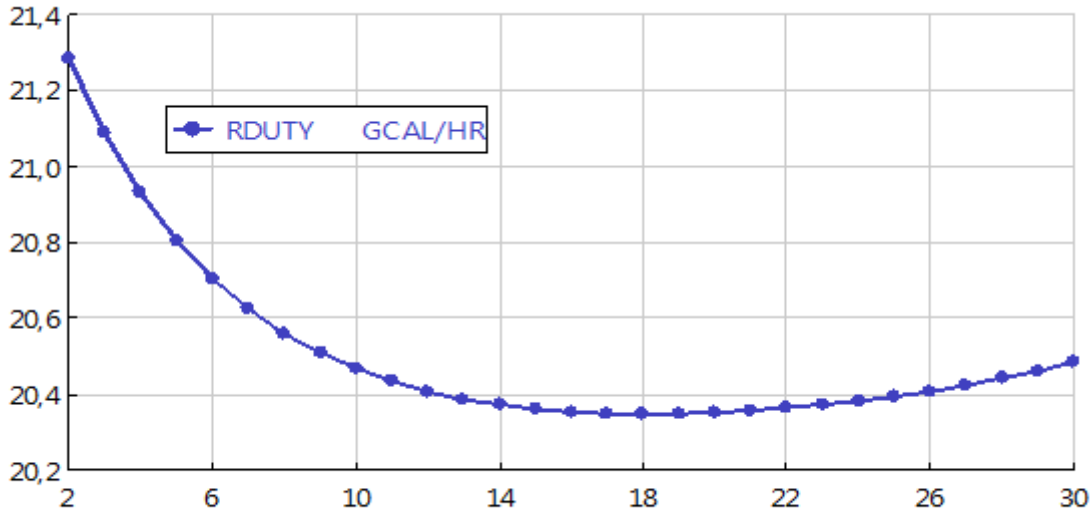

Figure 4. The graph of the dependence of reboiler energy consumption on the feed stage. X-axis is the energy flow of the reboiler Gkal/s, Y-axis is feed stage.

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2.4. Flooding factor of the column.

In order to verify the flexibility of the real column in the production, the calculations must be carried out according to the plate-interval characteristics. According to this calculation, the flooding factor among plates are determined by the actual steam velocity where flooding stage is generated and the ratio among steam velocity, and also the maximum flooding factor for the entire column. The diameter of the column for given flow is 5.8 meters, and flooding factor calculated in accordance with this diameter is presented in **Figure 5**.

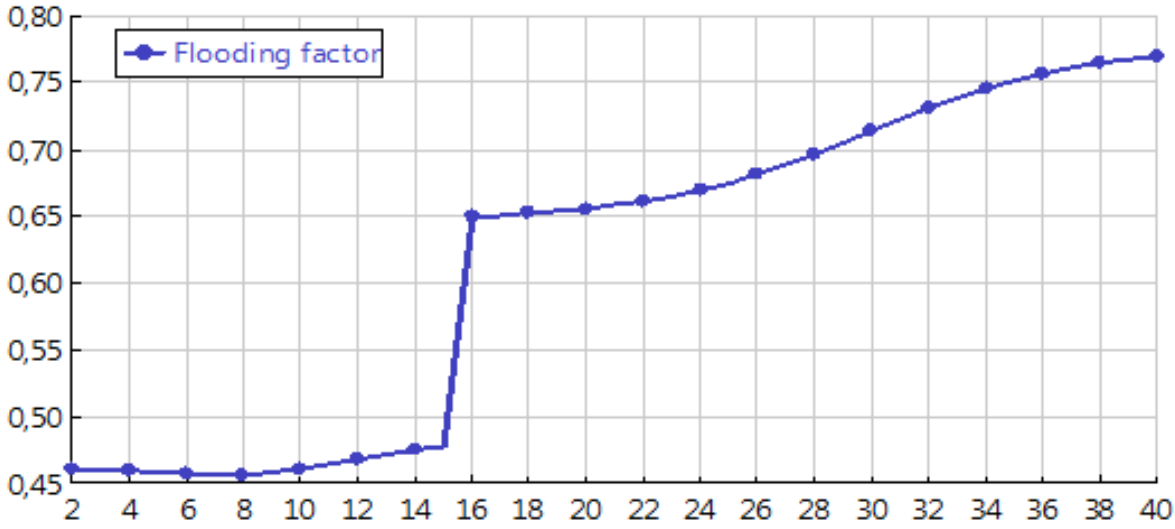

Figure 5. The results of calculating the flooding factor of the propane / butane mixture separation column in the Aspen plus program. X-axis is the number of plates, Y-axis is flooding factor.

3. Modeling results

Conditionally, We define the compositions of the feed substances Z, the distillate composition XD, and the substance composition of the bottom stream XB (all of which are given in propane molar proportions). According to **Table 3**, the XB distillate (DIST) and the bottom stream (BTM) are 99.3 and 0.4 respectively. 24 MW of medium pressure steam is as a heating energy during the separation, and cooling energy is cold water, which requires -24 MW of energy. Apart from that, the modeling results reveal CO2 emissions of about 5,600 kg /s to the atmosphere during the process of fractionation of this compounds.

Table 3. Modeling results by Soave-Redlich-Kwong thermodynamics

	BTM	DIST	FEED
Propane, kmol/s	9.80	1142.20	1152
Butane, kmol/s	2440.20	7.80	2448
Propane, mol %	0.40	99.30	0.32
Butane, mol %	99.60	0.70	0.68
Molar flow, kmol/s	2450	1150	3600
Temperature	81.33	40.36	48.85
Pressure, atm	13.45	13.17	20.26

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Conclusion

The results of the calculation indicate that use of modeling by computer software is an important tool for Engineers in calculating production processes and anticipating the needed factors. Selected modeling method is capable of providing the manufacturer with the ability to design a more efficient processing mechanism and reduce the CO2 emissions.

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