FRACTIONATION OF OIL MIXTURE INTO JET AND DIESEL FUEL. SIMULATION AND OPTIMIZATION IN CHEMCAD

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Abstract. The jet and diesel fuels production line has been simulated using the universal simulating program ChemCad. The choice of the rectification process calculation module was substantiated. The Grayson-Streed and Lee Kesler models were used for the calculation of the thermodynamic system and the phase equilibrium of the multicomponent mixture. The model of an oil mixture distillation unit for jet and diesel fuels production has been developed. The temperature profile of the column was obtained; the optimization problem was solved by finding the minimum number of trays in the distillation column. As a result, the optimal reflux ratio and optimal feed tray were defined, allowing to minimize energy consumption. The energy balance of the distillation column has been determined and calculated.

Keywords: scheme, modeling, separation, jet fuel, diesel fuel.

1. Introduction

Diesel and jet fuels are the liquid products of petroleum refining, which are used as fuel in internal combustion engines. This type of fuel is derived from kerosene-gas-oil fractions of direct oil distillation.[1] This fuel consists of a mixture of alkanes, cycloalkanes, aromatic hydrocarbons, and their derivatives. Diesel fuel is the most common type of fuel used in various industries and households. All trucks, tractors, road vehicles, agricultural machinery, rail transport use this type of fuel. Jet fuel is widely used in aviation.[2-3]

Since crude oil and petroleum products are a multicomponent mixture of hydrocarbons and heteroatomic compounds, it is impossible to use conventional distillation methods to divide them into individual compounds with well-defined physical properties, including the boiling point at a given pressure. Usually, crude oil and petroleum products are separated by distillation into individual components, each of which is a less complex mixture. Such components are called fractions or distillates. Under laboratory or industrial conditions, individual oil fractions are distilled off with a gradual increase in boiling point. Therefore, oil and its fractions are characterized not by the boiling point, but by the temperature limits of the beginning of boiling and the end of boiling.[4-6]

The main mass transfer process of oil refining in the industry is crude oil fractionation in distillation columns, where different fuel fractions are distilled, which are then used for the production of commercial fuels (gasoline, jet, and diesel fuels) and fuel oil, which is used either as a component of boiler fuel or as a raw material for further deep processing.[7-8] The obtained broad fuel fractions are directed for secondary refining or fed to be separated in order to obtain fuel components.[9-10]

In order to obtain a high-quality product, it is important to have not only quality crude oil but also modern technological equipment for processing. Continuous modernization of oil refinery equipment can significantly improve the quality of resulting products. With the modern development of computer technology and the availability of simulating programs, simulation of petroleum fuel production processes is becoming increasingly important. The obtained results allow to significantly reduce the operating time of equipment and the cost of technological processes.[11]

This is just a reason why the simulation of the jet and diesel fuels production line for using the ChemCad simulating program, and the application of modern thermodynamic models for the calculation of rectification processes are topical issues.[12-14]

When modeling petroleum rectification processes in ChemCad, the correct choice of the model for calculating the rectification process of multicomponent systems is an important task. There are three possible models: Tower distillation column (TOWR), Rigorous distillation column (SCDS), and Tower plus (TPLS). To make the right choice it is necessary to analyze the qualitative and quantitative composition of compounds involved in the process.[15] The choice depends on the

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phase composition of the compounds and the presence or absence of chemical reactions in the column.[16-19]

The next important step in the simulation of the multicomponent systems rectification is the choice of thermodynamic model. Toth[20] presents a number of fundamental equations of state for modeling the phase transition "liquid-gas", which satisfy the conditions of the critical point and can be given as the dependence of the thermodynamic potential on its own variables. Such equations are used to calculate thermodynamic systems and phase equilibrium of hydrocarbons and hydrocarbon mixtures.[21-23]

This publication aims to increase the efficiency of rectification process management by improving the current module (TOWR) due to minimizing energy consumption and applying the optimization problem.

To achieve this aim, it is necessary to solve the following tasks:

– to develop a calculation algorithm and choose a mathematical model for the calculation of the distillation column in order to obtain jet and diesel fuels;

– to investigate the effectiveness of the selected model integration on the example of the installation for the separation of the multicomponent mixture "jet fuel – diesel fuel";

– based on the simulation results of the ChemCad program for the separation process of multicomponent mixture "jet fuel – diesel fuel"" to increase the efficiency of multicomponent mixtures fractionation by minimizing energy consumption and applying the optimization problem.

2. Experimental

To choose the right thermodynamic model, it is necessary to consider the molecules of the studied multicomponent mixture as an aggregate of functional groups. In such a case, the thermodynamic properties of pure liquids can be calculated as the sum of the group components, and the thermodynamic properties of a large number of liquids are adjusted due to the smaller number of parameters characterizing the contributions of individual groups.

For the multicomponent jet-diesel mixture, calculations can be made using the Grayson-Streed and Lee Kesler models.[13-14]

The Grayson-Streed modified Chao-Seader model is primarily applicable to the systems of non-polar hydrocarbons. It is good for modeling hydrocarbon units, depropanizers, debutanizers, or reformer systems.

The approximate range of its applicability is as follows:

Temperature Range	Pressure Range
0 F to 800 F	<3000 psi
(255 K to 703 K)	(<20000 kPa)

The correlation can also be applied down to the lower temperature limit of the original Chao-Seader work ($T_r = 0.5$ for hydrocarbons except for methane) and down to −100 F for hydrogen and methane.

Hydrocarbon liquid solutions are considered to be regular solutions in this correlation. The liquid phase pure species fugacities are derived from Grayson-Streed's corresponding state option. Vapor phase mixture fugacity coefficients, as well as vapor compressibilities, are based on the Redlich-Kwong equation of state.

$$K_i = \frac{y_i}{x_i} = \frac{\eta_i^0 \gamma_i}{\phi_i} \tag{1}$$

The formulas of the Grayson-Streed model according to the coefficient of activity take the following form:

$$\ln_{\gamma i} = \frac{V_i(\delta_i - \overline{\delta_i})^2}{RT} \tag{2}$$

$$\overline{\delta_i} = \frac{(\Sigma x_i V_i \delta_i)}{\Sigma x_i V_i} \tag{3}$$

Fugacity coefficient in a vapor mixture:

$$z = \frac{1}{(1-h)} - \frac{A^2}{B} * \left(\frac{h}{(1+h)}\right) \tag{4}$$

$$h = \frac{BP}{z} \tag{5}$$

$$\ln\Phi_i = (z-1) * \frac{B_i}{B} - \ln(z - BP) -$$

$$- \frac{\alpha^2}{B}\left(\frac{2A_i}{A} - \frac{B_i}{B}\right) * \ln\left(1 + \frac{BP}{z}\right) \tag{6}$$

Numerical values are given by several authors.[16-18]

The Lee-Kesler enthalpy model is good for hydrocarbon systems. The general form of Lee-Kesler (LK) EoS is:[19]

$$z^{(i)} = \frac{p_r V_r}{T_r} = 1 + \frac{B}{V_r} + \frac{C}{V_r^2} + \frac{D}{V_r^5} + \cdot$$

$$+ \frac{c_4}{T_r^3 V_r^2} * \left(\beta + \frac{\gamma}{V_r^2}\right)\exp\left(\frac{-\gamma}{V_r^2}\right) \tag{7}$$

where, p_r is reduced pressure, p/p_c; p is pressure; p_c is pseudocritical pressure; $V_r = p_c V/RT_c$; V is molar volume for simple fluid or heavy reference fluid (n-octane); R is the gas constant; T_r is reduced temperature, T/T_c; T_c is pseudocritical temperature; T is the temperature; b1, b2, b3, b4, c1, c2, c3, c4, d1, d2, β, γ are constants, which can be obtained according to the API Databook.[24]

Through liquid-valor equilibrium calculation, the composition of each phase can be determined. Then, the pseudocritical parameters Tc and pc can be calculated by certain EoS mixing rules. By setting the variable Vr as the unknown value, Eq. (7) can be solved by Newton iteration algorithm.

Enthalpy departure:

$$\frac{H - H^*}{RT} = T_r \left[Z - 1 - \frac{b2 + 2b3/T_r + 3b4/T_r^2}{T_r V_r} - \right.$$

$$\left. - \frac{c2 - 3c3/T_r^2}{2T_r V_r^2} + \frac{d2}{5T_r V_r^3} + 3E \right] \quad (8)$$

where:

$$E = \frac{c4}{2T_r^3 \gamma} \left[\beta + 1 - (\beta + 1 + \frac{\gamma}{V_r^2}) \exp\left(-\frac{\gamma}{V_r^2} \right) \right]$$

$$(9)$$

Thus, the Grayson-Streed (for phase equilibrium) and Lee Kesler (for enthalpy) models can be used to simulate the separation process of a multicomponent mixture, such as "jet fuel – diesel fuel".

Fig. 1 shows a model of the main technological unit of the multicomponent mixture rectification in order to obtain jet and diesel fuels, which was developed in the ChemCad Universal Modeling Program (UMP).

This technological unit operates as follows: the original multicomponent mixture (stream 1) is fed to the feed tray of the distillation column (1column), where it is separated into the overhead product (stream 2) and the bottom product (stream 3). The reflux condenser (2heat exch) condenses and cools the product to 303 K. Stream 4 is jet fuel. The lower product (stream 3) from the column (1column), enters the cooler (3heat exch). Stream 5 is a diesel fuel cooled to 303 K.
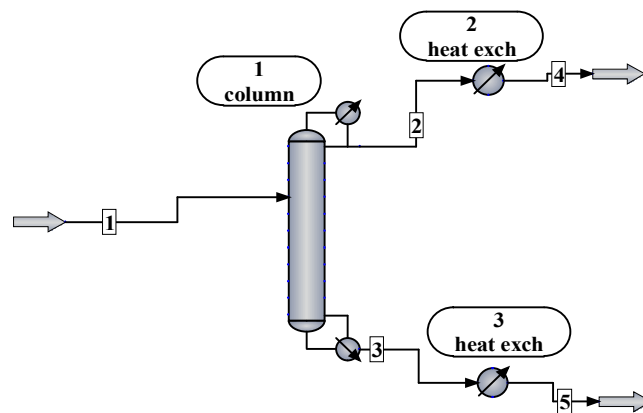

Fig. 1. Model of the technological unit of the multicomponent mixture rectification in order to obtain jet and diesel fuels, developed in ChemCad UMP

Devices: 1column – distillation column (TOWR module); 2heat exch – reflux condenser (HTXR module); 3heat exch – cooler (HTXR module). Streams: 1 – the original multicomponent mixture; 2 – vapors of overhead product (jet fuel); 3 –bottom product (diesel fuel); 4 – condensate of the overhead product at the reflux condenser outlet; 5 –diesel fuel at the cooler outlet

Table 1 shows the chemical composition of the multicomponent mixture, which enters the distillation column in order to obtain jet and diesel fuels. A process worksheet for the fractionation of the mixture is given in Table 2.

Table 1. The chemical composition of the multicomponent mixture, entered for separation to obtain jet and diesel fuels

Component	Gross-formula	Weight part, %	Boiling point (1 atm), K
1	2	3	4
Toluene	C_7H_8	3.5	383.6
Octane	C_8H_{18}	2.4	398.52
***p*-Xylene**	C_8H_{10}	1.0	411.3
***m*-Xylene**	C_8H_{10}	1.7	412.1
2-Methyloctane	C_9H_{20}	1.0	415
3-Ethylheptane	C_9H_{20}	1.1	416
3-Methyloctane	C_9H_{20}	0.9	417
***o*-Xylene**	C_8H_{10}	2.4	417.4
Cyclooctane	C_8H_{16}	2.7	422
Nonane	C_9H_{20}	1.9	424
Cumene	C_9H_{12}	2.3	425
Mesitylene	C_9H_{12}	1.0	438
Decane	$C_{10}H_{22}$	4.1	447
1-Methyl-4-isopropylbenzene	$n\text{-}C_{10}H_{14}$	3.1	450
N-butylbenzene	$C_{10}H_{14}$	4.9	456
cis-Decalin	$C_{10}H_{18}$	2.7	467.6
Undecane	$C_{11}H_{24}$	1.9	469
N-butylCycHexane	$C_{10}H_{20}$	4.1	474

Continuation of Table 1

1	2	3	4
Tetralin	$C_{10}H_{12}$	3.3	480
1,4-Diphenylbenzene	$C_{18}H_{14}$	1.2	486
Dodecane	$C_{12}H_{26}$	3.1	489
Naphthalene	$C_{10}H_8$	5.2	491
Tridecane	$C_{13}H_{28}$	3.1	507
2-Methylnaphthalene	$C_{11}H_{10}$	1.0	514.5
1-Methylnaphthalene	$C_{11}H_{10}$	4.8	518
Tetradecane	$C_{14}H_{30}$	3.0	526.6
Diphenyl	$C_{12}H_{10}$	1.6	528
Diphenylmethane	$C_{13}H_{12}$	2.3	537
Pentadecane	$C_{15}H_{32}$	4.2	543.7
Acenaphthene	$C_{12}H_{10}$	1.5	552
Hexadecane	$C_{16}H_{34}$	3.6	559.9
Fluorene	$C_{13}H_{10}$	3.3	568
Heptadecane	$C_{17}H_{36}$	2.5	575
Octadecane	$C_{18}H_{38}$	3.1	590
Nonadecane	$C_{19}H_{40}$	2.3	603
Phenanthrene	$C_{14}H_{10}$	1.5	613
Anthracene	$C_{14}H_{10}$	1.3	613
Eicosane	$C_{20}H_{42}$	1.7	616
Triphenylmethane	$C_{19}H_{16}$	1.7	632
Pyrene	$C_{16}H_{10}$	1.0	677
Chrysene	$C_{18}H_{12}$	1.0	721

Table 2. Process worksheet

Parameter	Units	Value	Permissible variation
Column inlet temperature	K	438	±5
Pressure in the feed part of the column	atm	1.1	±0.1
Mixture consumption at the column inlet	kg/h	15000	±100
Cooling temperature of the overhead product	K	303	±5
Cooling temperature of the bottom product	K	303	±5

3. Results and Discussion

When simulating, the energy balance of the process depicted in Fig. 1 was analyzed. The equation of the heat balance is:

$$Q_{f.s.1} + Q_{1C} + Q_{2HTXR} + Q_{3HTXR} + Q_{1R} =$$
$$= Q_{p.s.4} + Q_{p.s.5} + Q_{loss} \qquad (10)$$

$Q_{f.s.1}$ – feed stream heat duty (stream 1)

Q_{1C} – condenser heat duty (1 column)

Q_{2HTXR} – heat exchanger heat duty (2 heat exch)

Q_{3HTXR} – heat exchanger heat duty (3 heat exch)

Q_{1R} – reboiler heat duty (1 column)

$Q_{p.s.4}$ – product stream heat duty (stream 4)

$Q_{p.s.5}$ – product stream heat duty (stream 5)

Q_{loss} – heat loss

As can be seen from the equation, to minimize energy costs it is necessary to reduce the amount of heat in the cube of the column (reboiler) and in its upper part (condenser).

To do this, it is necessary to optimize the number of trays, the number of the feed tray, and the reflux. In other words, the result of simulation would be obtaining such numerical data of the above parameters, at which the energy costs of the process will be minimal.

Let's start the calculation of the technological unit model of the multicomponent mixture rectification process in order to obtain jet and diesel fuels, developed in ChemCad UMP (Fig. 1). As a result of the simulation, we obtain the temperature profile of the column (Fig. 2). As can be seen from Fig. 2, the temperature increases along with the height of the column from tray No.1 (top tray) to tray No. 24 (bottom tray). The curve is smooth, without stagnant zones both in temperature and in the profile of the column. That is, 24 trays are enough to separate this mixture.
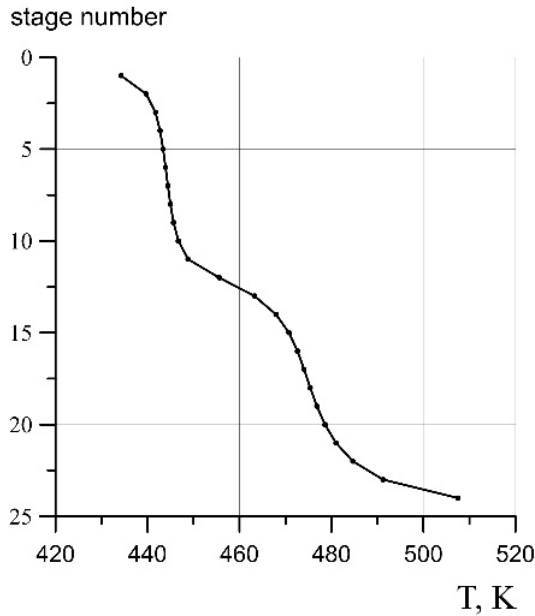
stage number

Fig. 2. The temperature profile
of the column

The next step is solving the optimization problem. Let us optimize the operation mode of the technological unit of the multicomponent mixture rectification process in order to obtain jet and diesel fuels by minimizing the number of trays of the distillation column. The criterion of optimality is the number of distillation column trays. Next, we specify the process independent variables, which will be used as search values in the optimization problem. This will be the reflux ratio and the bottom product temperature. We will impose constraints on them:

0.1 <reflux ratio <10

373 K <bottom product temperature <673 K

The established limits correspond to the characteristics of the multicomponent mixture rectification process in order to obtain jet and diesel fuels. The results of solving the optimization problem:

SQP Iteration 1
X[0] = 6.00000e-001
X[1] = 9.14670e+002

Objective Function (FO) = 2.40000e+001

Constraint Values (FC):
FC[0] = 5.00000e-001
FC[1] = 9.40000e+000
FC[2] = 2.43000e+002
FC[3] = 2.97000e+002
L40 X3MAX = 0.

Norm of Lagrangian Gradient = 0.00000e+000

Final Results:
Independent Variables in User Specified Engineering Units:

	Initial Value	Final Value
Reflux ratio	X[0] =	6.000000e-001
Bottom product temperature	X[1] =	2.350000e+002
Objective Function	2.400000e+001	2.400000e+001

No. of SQP iterations = 1
No. of function calls = 5

One can see that the rectification unit, shown in Fig. 1, is set to the optimal mode. The reflux ratio is 0.6 and the temperature in the cube of the column is 508 K.

The next step: the selection of a feed tray, the supply of feed on which would give the lowest energy costs. Fig. 3 shows the dependence of the heat amount consumed in the upper (*curve* 1) and bottom (*curve* 2) part of the column from the feed tray. As can be seen from Fig. 3, both the first and the second curves pass through a certain minimum value.
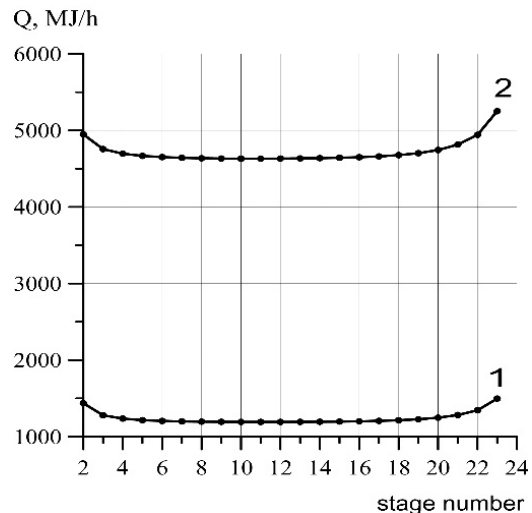

Fig. 3. Amount of heat consumed
in the upper (*curve* 1) and bottom (*curve* 2) part
of the column *vs.* feed tray

To visualize the optimal feed tray, we present a graph of the heat amount in the bottom part of the column *versus* the range of feed trays No. 8–14 (Fig. 4a) and a graph of the heat amount in the upper part of the column on the same range of feed trays (Fig. 4b). As can be seen from Fig. 4 the optimal power tray is tray No. 11.

Therefore, the operating parameters of the simulated distillation unit after optimization and, as a consequence, minimization of the energy amount are given in Table 3.

The energy amount spent for the rectification process we calculate in accordance with the energy balance (Eq. 10). Table 4 shows the values of input and output energy calculated during simulation.
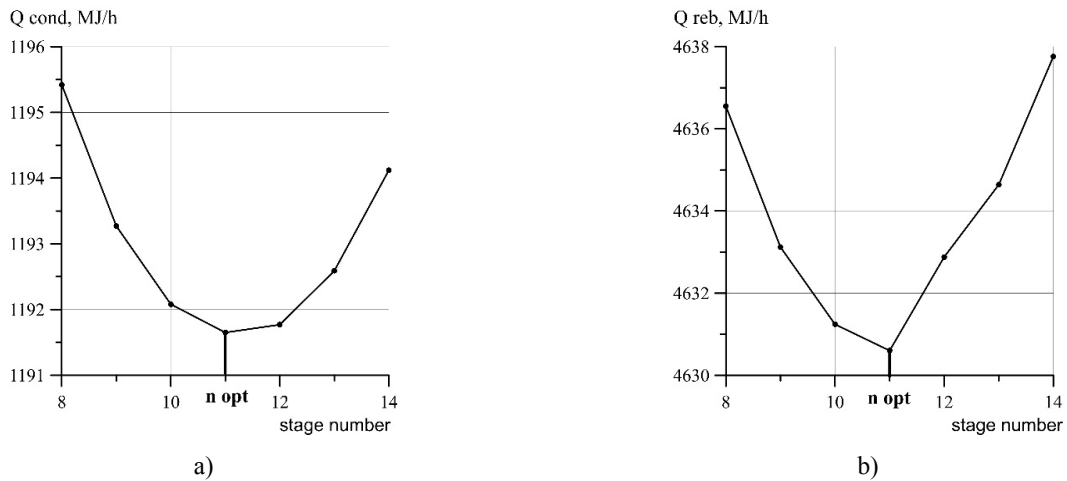
Fig. 4. Determination of the optimal feed tray depending on the heat amount
in the upper part of the column (a) and the bottom part of the column (b)

Table 3. Equipment summaries. TOWR Rigorous Distillation Summary

Parameters	Values
Equip. No	1
Name	column
No. of stages	24
1st feed stage	11
Top pressure atm	1.0000
Condenser type	1
Condenser mode	1
Condenser spec.	0.6000
Reboiler mode	3
Reboiler spec.	235.0000
Initial flag	6
Calc cond duty MJ/h	-1191.6465
Calc rebr duty MJ/h	4630.5938
Est. Dist. Rate (kmol/h)	45.6837
Est. Reflux rate (kmol/h)	27.4102
Est. T top K	431.7390
Est. T bottom K	508.0000
Est. T 2 K	478.6528
Cost estimation flag	1
Calc Reflux ratio	0.6000
Calc Reflux mole (kmol/h)	28.0736
Calc Reflux mass kg/h	3630.4897
Optimization flag	1

Table 4. Values of input and output energy calculated during simulation

Heat	Input, MJ/h	Output, MJ/h
$Q_{f.s.1}$	8792.936	–
Q_{1C}	1191.65	–
Q_{2HTXR}	3368.16	–
Q_{3HTXR}	4226.97	–
Q_{IR}	–4630.59	--
$Q_{p.s.4}$	–	6355.317
$Q_{p.s.5}$	–	6591.959
Q_{loss}	–	1.85
TOTAL $\sum Q$	**12949.126**	**12949.126**

Thus, according to Table 4, the calculated energy consumption will be minimal under optimized operation of the column.

So, the separation of the multicomponent mixture into overhead and bottom products (jet fuel and diesel fuel, respectively) is achieved with the minimum amount of energy consumed. The quantitative and qualitative compositions of obtained fuels are given in Table 5.

Therefore, the high-quality separation of the multicomponent mixture into jet and diesel fuels is possible after simulation, process optimization and minimization of energy consumption.

Table 5. Chemical composition of jet and diesel fuels obtained after separation of the multicomponent mixture in the rectification column

Component	Weight part, %	Weight overhead part, %	Weight bottom part, %
Toluene	**3.5**	**9.24**	**6.45e-009**
Octane	**2.4**	**6.34**	**1.41e-008**
p-Xylene	**1.0**	**2.64**	**3.316e-006**
m-Xylene	**1.7**	**4.49**	**6.28e-006**
2-Methyloctane	**1.0**	**2.64**	**9.28e-007**
3-Ethylheptane	**1.1**	**2.91**	**8.96e-007**
3-Methyloctane	**0.9**	**2.38**	**1.18e-006**
o-Xylene	**2.4**	**6.34**	**4.17e-005**
Cyclooctane	**2.7**	**7.13**	**0.00018**
Nonane	**1.9**	**5.02**	**9.95e-006**
Cumene	**2.3**	**6.07**	**0.0003**
Mesitylene	**1.0**	**2.63**	**0.005**
Decane	**4.1**	**10.73**	**0.023**
1-Methyl-4-isopropylbenzene	**3.1**	**7.29**	**0.34**
N-Butylbenzene	**4.9**	**8.71**	**1.88**
cis-Decalin	**2.7**	**2.9**	**2.11**
Undecane	**1.9**	**1.92**	**1.68**
N-ButylCycHexane	**4.1**	**7.83**	**1.33**
Tetralin	3.3	1.59	4.89
1,4-Diphenylbenzene	1.2	0.0001	1.96
Dodecane	3.1	0.17	5.01
Naphthalene	5.2	0.92	7.89
Tridecane	3.1	0.0009	5.08
2-Methylnaphthalene	1.0	0.0006	1.64
1-Methylnaphthalene	4.8	0.005	7.86
Tetradecane	3.0	2.16e-006	4.91
Diphenyl	1.6	8.85e-006	2.62
Diphenylmethane	2.3	5.68e-007	3.77
Pentadecane	4.2	9.18e-009	6.88
Acenaphthene	1.5	3.71e-008	2.46
Hexadecane	3.6	1.13e-011	5.89
Fluorene	3.3	9.55e-008	5.4
Heptadecane	2.5	5.49e-014	4.09
Octadecane	3.1	1.43e-016	5.08
Nonadecane	2.3	1.4e-016	3.77
Phenanthrene	1.5	1.83e-016	2.46
Anthracene	1.3	1.83e-017	2.13
Eicosane	1.7	1.83e-018	2.78
Triphenylmethane	1.7	1.83e-019	2.78
Pyrene	1.0	1.83e-020	1.64
Chrysene	1.0	1.83e-021	1.64
TOTAL	**100**	**100**	**100**

4. Conclusions

Using ChemCad UMP, a simulation has been developed based on the selected model for calculating the multicomponent mixture rectification process to obtain jet and diesel fuels, as well as Lee Kesler and Grayson-Streed models for calculating the thermodynamic system and phase equilibrium of this multicomponent mixture. As a result of the simulation, the temperature profile of the column was obtained, the optimization problem was solved by minimizing the number of trays. We obtained the optimal reflux ratio and the optimal feed tray, the supply of feed for which gives the minimum energy consumption. The energy balance of the rectification unit was calculated. The determined value of heat energy for the process is $\Sigma Q = 12949.126$ MJ/h. Under the conditions of this consumed energy, the high-quality separation of the multicomponent mixture into jet and diesel fuels can be achieved.

Thus, the obtained results allow to modernize the equipment by optimizing the process and minimizing the energy consumed for the process, which in turn will significantly reduce the operating time of the equipment and the cost of technological processes.

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МОДЕЛЮВАННЯ ТА ОПТИМІЗАЦІЯ В CHEMCAD ПРОЦЕСУ РОЗДІЛЕННЯ НАФТОВОЇ СУМІШІ НА РЕАКТИВНЕ ТА ДИЗЕЛЬНЕ ПАЛИВО

Анотація. *Наведено результати досліджень моделювання в універсальній моделюючій програмі ChemCad технологічної лінії виробництва реактивного та дизельного палив. Обґрунтовано вибір модуля розрахунку процесу ректифікації. Обґрунтований вибір моделі Grayson-Streed та Lee Kesler для розрахунку термодинамічної системи та фазової рівноваги даної багатокомпонентної суміші. Розроблена модель технологічного вузла перегонки нафтової суміші для виробництва реактивного і дизельного палив. Отримано температурний профіль колони, вирішено завдання оптимізації знаходженням мінімальної кількості тарілок у ректифікаційній колоні. У результаті оптимізації отримано оптимальне флегмове число та оптимальну кількість тарілок живлення, подачу живильної суміші, що дає можливість мінімізувати споживання енергії. Встановлено та розраховано енергетичний баланс ректифікаційної колони.*

Ключові слова: *схема, моделювання, розділення, реактивне паливо, дизельне паливо.*