Program for calculating the technological and structural characteristics of plate and packed distillation columns for separating two, multicomponent mixtures and isotopes

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Abstract. The article describes the developed and software implemented methods for calculating the technological and structural characteristics of plated and packed distillation columns for separating two-component, multicomponent and isotopic mixtures. The results of the verification of the methods are presented. A good convergence of the calculation results with the known literature data is shown.

1. Introduction

Rectification is widely used in the nuclear industry. Currently, many enterprises are implementing measures to improve this technology and hardware design in terms of energy saving and resource saving, increasing the efficiency of this process. These measures were of particular importance in the creation or modernization of installations for the separation of substances with similar physicochemical properties and isotopes, where, due to the small single separation coefficient, the processes are carried out in multistage counterflow columns. To solve these problems, it is advisable to use the possibility of determining the technological and structural parameters of distillation columns by calculation. At the enrichment plants, there is a global replacement of obsolete rectification columns with new ones and optimization of their operating modes. In addition to solving the above problems, it becomes urgent to improve the methods for calculating the technological and structural parameters of distillation columns [1-4]: increasing the speed and accuracy of computer-assisted calculations, ensuring the versatility of methods and software for calculating different types of columns and contact devices (CD), using new approaches to determining these parameters and automatized search for the optimal implementation of the enrichment plant.

In this regard, the goal of this work was to create and verify universal software for automatized calculation of technological and structural parameters and design of distillation columns.

2. Object of research

The object of the research was rectification columns (figure 1) with plate-shaped and packed contact devices, designed to separate two, multicomponent and isotopic mixtures. The separated mixture F with the concentration of the low boiling component (LBC) x_f, enters the column. The counterflow of the phases is created by a still-evaporator (1), where steam is continuously formed and the bottom liquid W goes out, enriched in a high boiling component (HBC) to a concentration x_w, also there is a condenser

(2), in which the rising steam is cooled, forming a distillate P, enriched in LBC to a concentration x_p. Part of the distillate stream P is fed to the top of the column for reflux in the form of reflux Φ. The initial data for the calculation are the technological task, physical-chemical and thermodynamic properties of the components of the mixture to be separated, which are specified by the user or selected from databases.

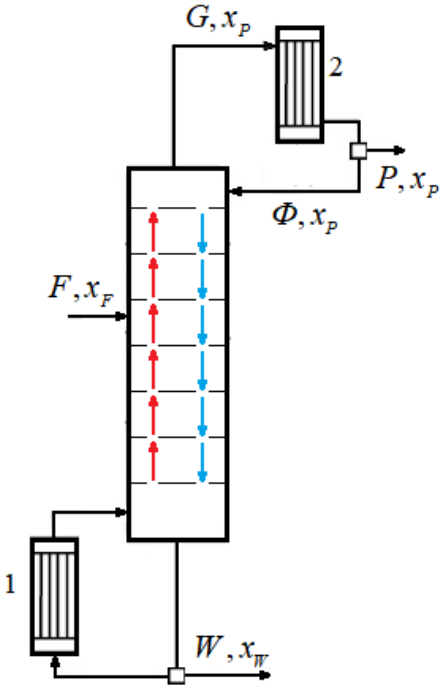

Figure 1. Distillation column

3. Methods for calculating the rectification columns

The well-known techniques [2-5] with the following assumptions were used as the basis for calculating the technological and structural parameters of the distillation columns:

1. There are no heat losses from the column to the environment.
2. Feed enters the column at the boiling point of the mixture.
3. The heat of mixing of the mixture components at the theoretical stages equals to zero.
4. The column pressure is constant.
5. The molar heat of vaporization of the mixture components at the same temperature is approximately the same.
6. The concentration of the target component in the vapor rising from the upper contact device of the column does not change in the reflux condenser.
7. Upon evaporation of the bottom liquid, the concentration of the target component in the vapor rising to the first CD does not change.

These techniques can be used to calculate the technological and structural characteristics of plated and packed distillation columns. They are based on a block approach, which makes it possible to quickly modernize each block of the program separately when new empirical dependencies and new approaches to calculation appear.

Technological calculation for plated and packed columns is carried out in the same way and begins with the input of the initial data. Then, preliminary calculations are carried out, during which the entered data is approximated. Further, the mass concentrations of the separated components are converted into molar ones, and the flow of the distillate, the distillation residue, and the minimum reflux ratio $R_{\min}$ are calculated. The working reflux ratio is calculated by the formula:

$$R = R_{min} \cdot \beta , \qquad (1)$$

where β – excess reflux ratio, the value of which ranges from 1.1 to 6.

The calculation of the number of theoretical stages (NTS) is carried out in an analytical way, in which for each step it is necessary to use a computer to calculate the strengthening and extracting sections:

$$\begin{cases} y_f = \sum_{n=0}^{m} a_n \cdot x^n \\ y_{str.s} = \dfrac{R}{R+1} \cdot x + \dfrac{x_P}{R+1} \end{cases}, \quad (2)$$

$$\begin{cases} y_f = \sum_{n=0}^{m} a_n \cdot x^n \\ y_{ex.s} = \dfrac{R+f}{R+1} \cdot x - \dfrac{f+1}{R+1} x_W \end{cases}, \quad (3)$$

where a_n – coefficient of the polynomial obtained by approximating the *x, y* points of the phase equilibrium curve, m – maximum degree of a polynomial.

To determine the optimal reflux ratio R and NTS, it was proposed to calculate the dependence of $N(R+1)$ on R with a smaller step of change β (figure 2).

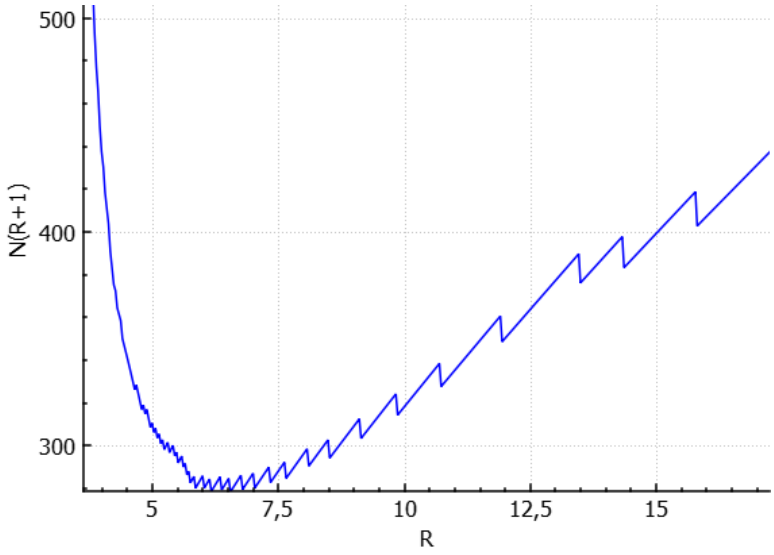

Figure 2. Dependence $N(R+1)$ on R

As a result, instead of a smoothed curve, a saw-tooth shape was obtained, the minimum values of which correspond to the minimum values of the reflux ratio with the same number of theoretical stages.

This made it possible to more accurately determine the NTS in the column and to abandon the use of empirical corrections in the calculations, which previously ranged from 5 to 25%.

The physical-chemical properties of the mixture are calculated automatically according to the polynomial dependence of each property on temperature.

Mass flows of steam in sections are calculated by the formulas:

$$G_{str} = (1+R)P \cdot \frac{M_{s_{str}}}{M_P}, \quad (4)$$

$$G_{ex} = (1+R)P \cdot \frac{M_{s_{ex}}}{M_P}, \quad (5)$$

where $M_{s_{str}}$ and $M_{s_{ex}}$ – average molar mass of steam in the strengthening and extracting sections, kg/kmol.

Mass flows of liquid in sections are calculated by the formulas:

$$L_{str} = RP \cdot \frac{M_{L_{str}}}{M_P}, \quad (6)$$

$$L_{ex} = L_{str} + F \cdot \frac{M_{L_{ex}}}{M_F}, \quad (7)$$

where $M_{L_{str}}$ and $M_{L_{ex}}$ – average molar mass of liquid in the strengthening and extracting sections, kg/kmol.

The volumetric flow rate of vapor and liquid in sections is calculated as the ratio of the mass flow rate to the corresponding density value. The thermal design of the column is carried out for the distillation still and condenser.

The design calculation for plated and packed columns is different. The initial data are the terms of reference and the results of the technological calculation.

Structural calculation of plated columns begins with automatic reading of the results of technological calculation and type CD from the technical assignment. Then the calculation of auxiliary complexes and the starting diameter of the column is carried out. The starting distance between the plates is selected. The height of the drain threshold, the hydraulic resistance of the plate, the interplate liquid carryover, and the velocity of the liquid in the overflow device are calculated. The final step is to calculate the number of actual plates and the column height.

In the calculation method, as a result of enumerating the possible diameters of the column and the distances between the plates, an operable CD is searched for, for this the following conditions are automatically checked:

1. The actual steam velocity in the column, taking into account its possible increase or decrease, should be within allowable minimum and maximum values.
2. Interplate liquid carryover must not exceed the limiting value.
3. The actual fluid velocity in the overflow devices must be less than the permissible one.

Structural calculation of packed columns is carried out in the same way, but using different formulas and working conditions, taking into account the design features of packed columns and the method of phase contact.

The developed calculation methods are software implemented in the Qt Creator cross-platform development environment with the help of the C ++ programming language.

4. Software interface

The program has three tabs: «Create Template», «Column Analysis» and «About». The first tab is designed to enter initial data and technical specifications for the calculation. The second tab is intended for obtaining graphical and numerical results of the calculation and automatically saving them to the database. The third tab contains only information about software developers.

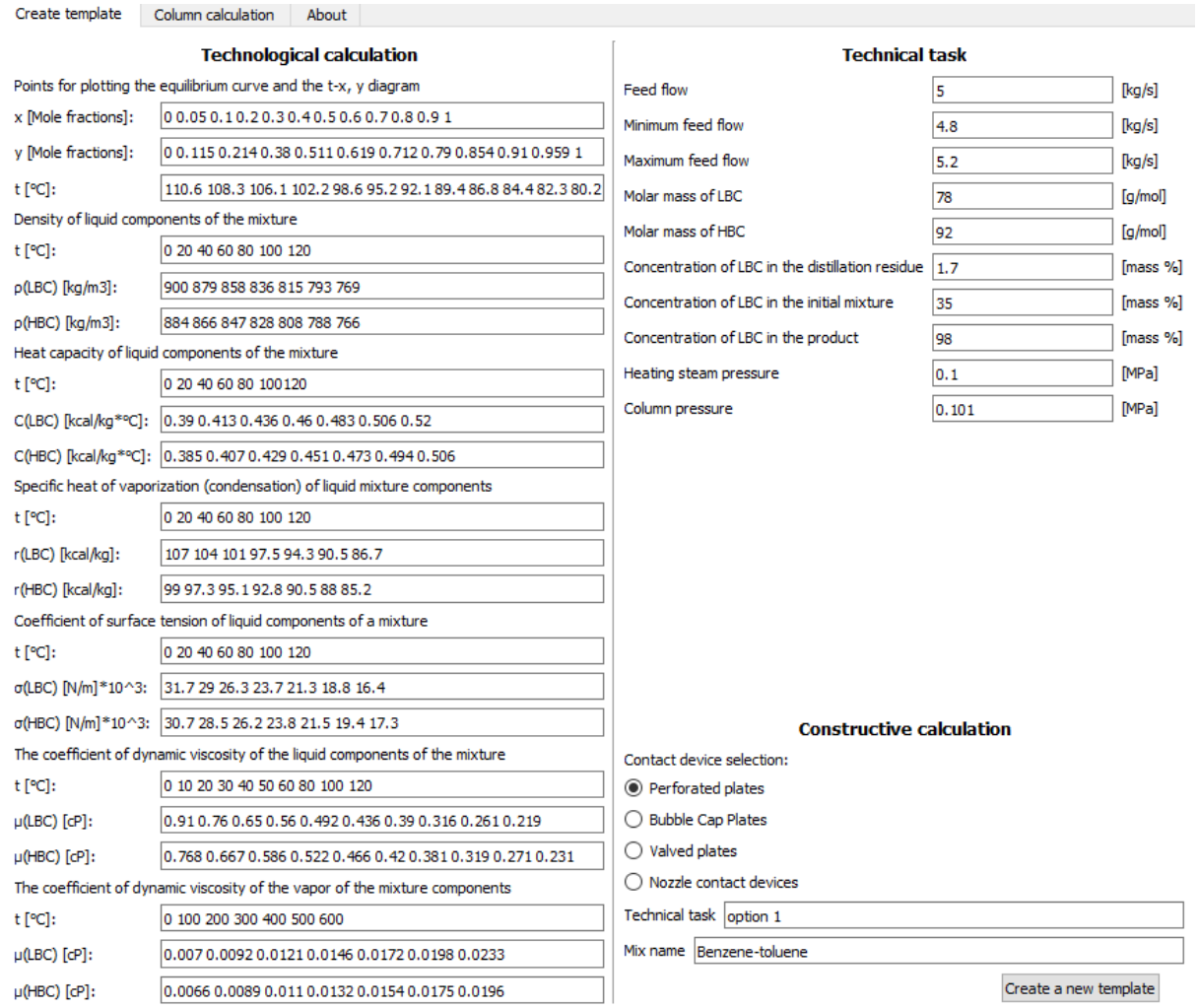

Figure 3. Initial data for verification

5. Verification of the mathematical model

With the help of the developed and software-implemented methods, the calculations of the technological and structural characteristics of the plated and packed columns for the benzene-toluene system were carried out. This system was chosen due to the lack of a data set for isotopic mixtures required for verification in the literature. The calculation conditions are shown above in the screenshot (figure 3). The calculation time was 3 s.

After the calculation, graphs of the main dependencies are displayed on the computer screen (figure 4–6). The numerical data of the calculation are automatically recorded in the database in the form of a text file. The main calculation results are shown in table 1.

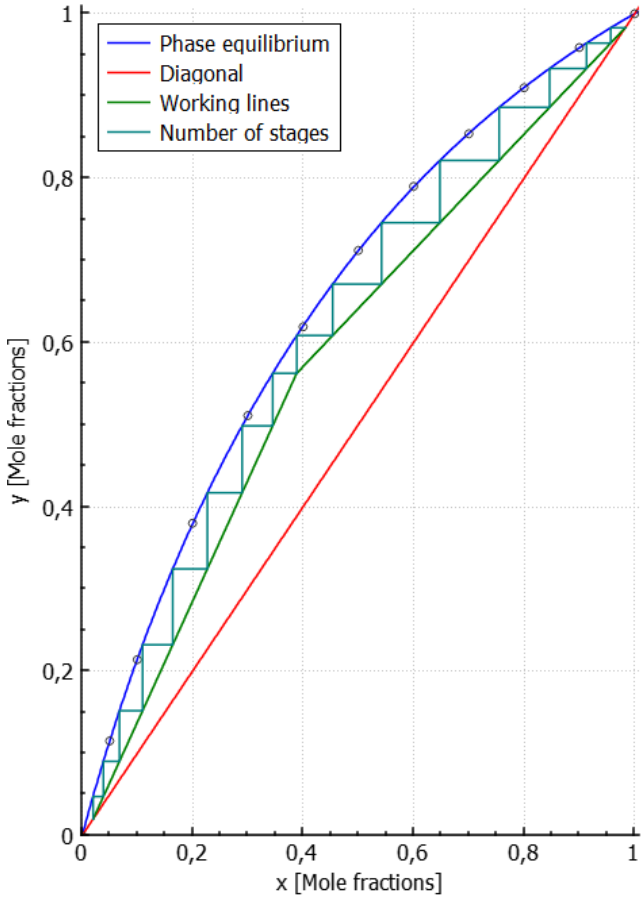

Figure 4. Diagram *x-y*

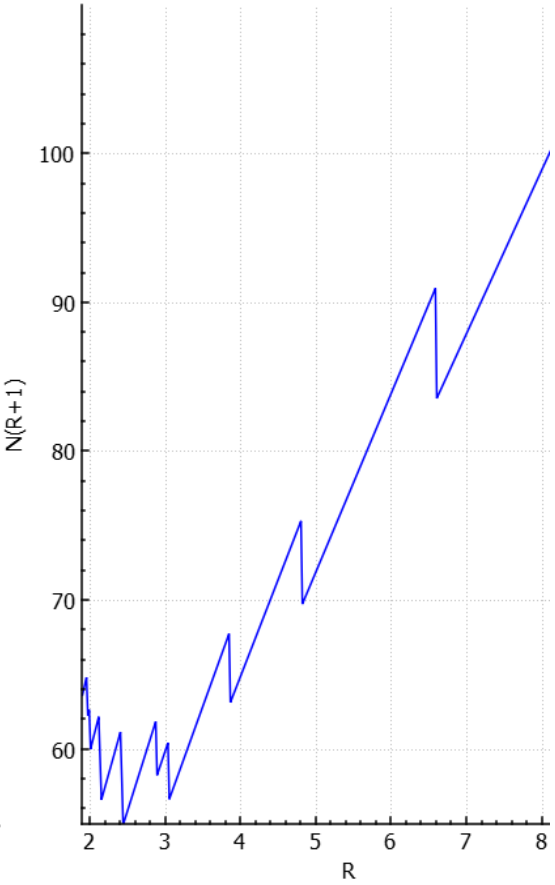

Figure 5. Dependence $N(R+1)$ on R

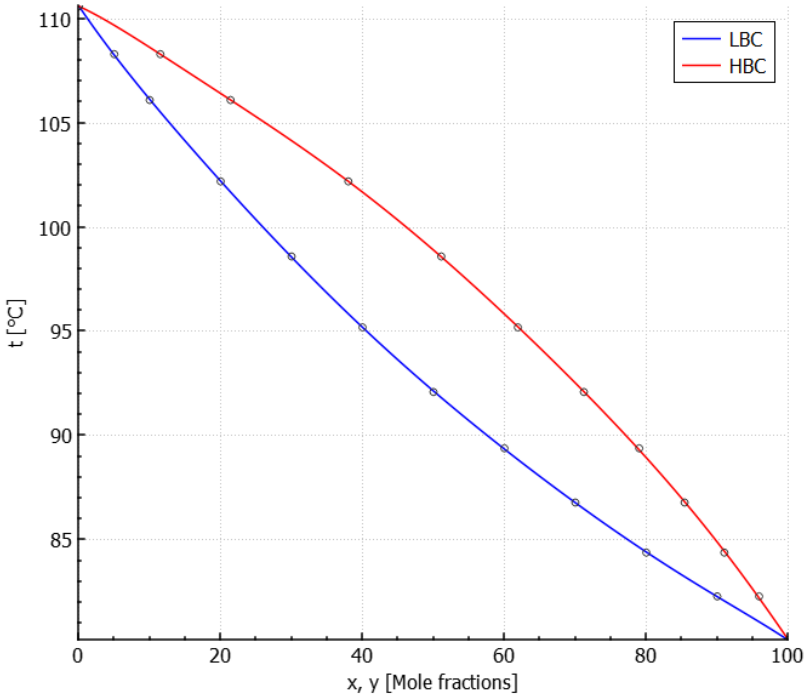

Figure 6. Diagram *t-x*, *y*

Table 1. Calculation results for plated and packed columns for separating benzene-toluene mixture

Value	Calculation results using the developed software	Calculation results [6]
Technological calculation		
Minimum reflux ratio, R_{min}	1.71	1.68
Optimum reflux ratio, R	2.45	2.1
NTS, N	17	22
Mass flows of steam in sections, G_S, [kg/s]	5.55; 5.87	5.58; 6.04
Mass flow of liquid in sections, G_L, [kg/s]	3.84; 9.29	3.84; 9.29
Structural calculation of the plate column		
Plate type	Perforated	Perforated
Plate design	TC-P	TC-P
Plate column diameter, D_p, [m]	1.6	1.8
Diameter of the holes in the plate, d_0, [mm]	8	8
Hole pitch, t, [mm]	15	15
Interplate distance, H_t, [m]	0.45	0.5
Number of valid stages	25	31
Plated column height, H_p, [m]	15	18
General hydraulic resistance, P_p, [Pa]	7650	8225
Structural calculation of packed column		
Nozzle type	Raschig rings	Raschig rings
Size of the nozzle [mm]	50x50x5	50x50x5
Packing column diameter, D_n, [m]	1.6	1.6
Packing column height, H_n, [m]	40	41
General hydraulic resistance, P_n, [Pa]	24500	25500

Comparative analysis of the results of technological calculation showed their good convergence. Consequently, these techniques make it possible to adequately calculate the technological and structural characteristics for plated and packed columns.

Most of the calculated values of technological parameters are the same. Differences appear only when determining the reflux ratio and the number of theoretical separation stages. In [6], the NTS was determined graphically, while the software values were obtained analytically by solving the equations of the equilibrium curve and working lines.

Due to the difference in NTS and the step of the reflux ratio β, the values of the reflux ratio are also different. As a consequence, the reflux-dependent parameters differ from the data [6].

The choice of the type of sieve plate TC-P and the diameter of the column was carried out by the author [4] on the basis of his experience and recommendations given in the literature, and the software selected them automatically and made it possible to determine the optimal option - the minimum diameter of the column at which it remains operational. The calculated data for packed column also have good convergence. Consequently, these techniques make it possible to adequately calculate the technological and structural characteristics for plated and packed columns.

6. Conclusion

1. Original methods have been developed for calculating the technological and design parameters of distillation columns with different CDs, which allow for a more accurate analytical determination of the reflux ratio, NTS separation, which made it possible to abandon the use of empirical NTS corrections in further calculations and more accurately determine all column parameters that depend on the reflux ratio and NTS.
2. It is shown that the use of a small step of changing the reflux excess ratio allows obtaining a more accurate form of the dependence of $N(R+1)$ on R, due to this, it is also possible to more accurately determine the optimal reflux ratio.
3. On the basis of the developed methods in the Qt Creator cross-platform development environment with the help of C ++ programming language, a universal software has been created that allows you to quickly carry out automated calculations of plated and packed distillation columns, as well as to select the optimal process parameters in accordance with the optimality criteria laid down in the calculation methods.
4. The software was verified for a benzene-toluene mixture. A good convergence of the calculation results with the known literature data is shown.
5. The implemented mathematical model, due to the underlying algorithms, speed and accuracy of calculations on a computer, allows calculations for systems with similar physicochemical properties and isotopes, in which the number of theoretical separation steps is much greater than in the example considered.

References

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