The improvement in technology of rectification column calculation

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Abstract. The task of automation and increasing the efficiency of calculating the parameters of the rectifying column for the needs of chemical production is being solved. Rectification is one of the most time-consuming chemical-technological processes responsible for the separation of liquid mixtures into practically pure components, which differ in boiling points, by repeated evaporation of the liquid and vapor condensation. The possibility of separation of the liquid mixture into its constituent components by distillation is due to the fact that the composition of the vapor formed above the liquid mixture differs from the composition of the liquid mixture under the conditions of the equilibrium state of steam and liquid. To select the optimal working conditions, it is necessary to take into account the heat consumption, temperature and pressure of the heat carrier - heating steam and cooling water, as well as the necessary dimensions of the columns and connecting elements with it by heat exchangers. All these factors are interrelated and depend, in particular, on the temperature and state of aggregation of the mixture supplied for separation. When calculating the processes of rectification, the compositions of liquids are usually given in mass fractions or percent, and for practical calculation it is more convenient to use the compositions of liquids and steam, expressed in molar fractions or percent. The software being developed will automate the calculation of distillation plants, which will increase the calculation speed. In most existing installations, rectification is not clear. The resulting components of light and oil distillates do not correspond to the required fractional composition, overgrowth of fractions is observed, some of the heaviest fractions of light diesel oil products fall into the bottom of the column, into fuel oil. Therefore, much attention is paid to the study and analysis of the operation of distillation columns, improving the methods of their calculation. The software created as a result of the project will be used directly by technologists, chemists and professors.

1. Introduction

The development of information systems and the creation of new information technologies lead to the emergence and growth of information components in all areas of society: in production, science, education, and medicine. Personal data processing systems, workstations based on personal computers are being improved.

In this series, computers and other electronic equipment occupy a special place, associated with their use as a tool for technological calculations and, as a result, optimization of an engineer. Using PCs as information machines can reduce the time required to prepare specific production projects, reduce
unproductive costs during their implementation, and eliminate the possibility of errors related to the human factor as much as possible.

Mathcad is the most widely used mathematical application for calculating rectification installations. This program has a wide range of multifunctional tools to solve problems using analytical, numerical and graphical methods, and is used to study the process of rectification of multicomponent mixtures.

At large chemical and oil refineries, powerful software HYSYS, PRO-II, CHEMCAD and others have recently been used to simulate production plants using the potential of which the most optimal operating conditions for individual stages and entire productions are selected.

Unfortunately, the use of these software packages in the educational process or other small enterprises is limited due to their high cost. Also, often the user does not need many tools that existing programs possess, but they need those that they do not possess.

To overcome the indicated difficulties, it is proposed to develop a software tool for automating the distillation unit calculation.

The relevance of this topic is that these calculations of the parameters of rectification plants are relevant for technologists, engineers and chemists in solving repeated typical problems.

2. Description of the installation technological scheme
Calculation of a distillation column is reduced to determining its main parameters - diameter and height. Both parameters are largely determined by the hydrodynamic regime of the column, which, in turn, depends on the speed and physical properties of the phases, as well as on the type and size of the plates.

The distillation column has a cylindrical body, inside of which contact devices in the form of plates or nozzles are installed. From bottom to top, the vapors move to the bottom of the apparatus from the boiler, which is located outside the column.

The steam passes through a layer of liquid on the lower plate, which we will take first, leading the numbering of plates conditionally from bottom to top.

Let \( x_1 \) be the concentration of the low-boiling component in the liquid feed mixture to be separated, and \( t_1 \) be the temperature of the mixture on the first plate. After the interaction of the mixture and the supplied steam, which has a higher temperature, partial evaporation of the liquid occurs on the first plate. Part of the low-boiling component passes into the steam, condenses and returns to the mixture the high-boiling component.

The evaporation of liquid on a plate occurs due to the heat of condensation of steam. The steam condenses and passes into a high-boiling component, the content of which in the steam entering the plate is higher than the equilibrium one with the composition of the liquid on the plate. If the heat of vaporization of the components of the binary mixture is equal, for the evaporation of 1 mol of the low-boiling component, it is necessary to condense 1 mol of the high-boiling component, the phases on the plate exchange equimolecular amounts of components.

On the second plate, the liquid has a composition \( x_2 \) containing more low-boiling component than on the first (\( x_2 > x_1 \)), and accordingly boils at a lower temperature (\( t_2 < t_1 \)). In contact with it, the vapor of composition \( y_1 \) is partially condensed, enriched with a low-boiling component and removed to an upstream plate having the composition \( y_3 > x_2 \).

So, the steam, which is almost pure at the outlet of the boiler, which almost completely passes into the vapor phase on the way of steam from the boiler to the top of the column.

Vapors condense in a water-cooled reflux condenser, and the resulting liquid is separated into distillate and reflux, which is sent to the top plate of the column. Therefore, using a reflux condenser in the column creates a downward flow of liquid. When the liquid reaches the bottom plate, it becomes an almost pure high-boiling component and enters the boiler, heated with dead steam or other coolant.

At a certain distance from the top of the column to the liquid from the reflux condenser, an initial mixture is attached, which enters the so-called feeding plate of the column.

In the upper part, greater strengthening of the low-boiling components should be ensured so that vapors are sent to the reflux condenser that are close in composition to the pure low-boiling component. In the lower part, remove the low-boiling components from the liquid as much as possible so that a
liquid similar in composition to the clean high-boiling component flows into the boiler. Accordingly, this part of the column is called exhaustive, in it either all the pairs coming from the column or only part of them corresponding to the amount of reflux returned to the column can be condensed. In the first case, the part of the condensate remaining after the separation of reflux is a distillate (rectified), or, the upper product, which, after cooling in the refrigerator, is sent to the distillate collector. In the second case, the non-condensed vapors in the reflux condenser are simultaneously condensed and cooled in the refrigerator, which in this embodiment serves as a condenser-cooler of the distillate. The liquid leaving the bottom of the column is also divided into two parts. One part, as indicated, is sent to the boiler, and the other - the remainder (bottom product) after cooling with water in the refrigerator is sent to the collection [7][8].

3. System design
Reference data for the calculation of the distillation unit: for each component of the mixture, it is necessary to enter into the database information on the density, viscosity, surface tension, diffusion coefficients, molar mass, saturated vapor pressure, melting temperature, specific heat of vaporization of substances entering the mixture at different temperatures, equilibrium compositions of the mixture. Input data: name of the mixture, plant capacity, composition of the initial mixture by low-boiling component, composition of the distillate by low-boiling component, composition of the residue by low-boiling component, input of a correction factor that takes into account the increase and narrowing of the fluid flow as a result of compression by the walls when approaching the drain wall [1] [4].

Direct calculation using reference and incoming information. The main stages of the calculation:

- calculation of the necessary concentrations of the initial mixture, distillate and still residue;
- calculation of the material balance of the rectification process;
- calculation of reflux-to-product ratio;
- calculation of volumetric steam flow;
- calculation of column diameter;
- calculation of column height;
- calculation of column hydraulic modes;
- thermic calculation of rectifying column;
- calculation of column thermal insulation.

![Figure 1. Physical model of the database of directories.](image-url)
To improve the quality and speed of development, the basic principles of software engineering were taken into account. The task of creating a database of mix directories was solved. The physical model of the database of directories is presented in figure 1 [3].

To automate the process of designing an information system, Case will be used - tools that facilitate mutual understanding between the customer and the developer, which helps prevent serious errors at the initial stages of design. At this stage, the diagrams were designed: use cases (figure 2), activities for the calculation process, sequences, cooperative diagrams [2].

![Use-Case Diagram](image)

**Figure 2. Use-Case Diagram.**

Setting up this software will be limited to installing it on a personal computer. The visual part of this software will be a set of forms that facilitate the input and perception of information.

4. Software implementation
When developing a software tool, all customer requirements were taken into account. For the convenience of using the system, a classic interface was developed, and the generally accepted color gamut was used (figure 3) [5] [6].

At the first start, the “Directories” and “Calculate” buttons will be unavailable, you need to connect the database, by default a window with the program folder opens, select in Microsoft Access. Next, in the main window of the program, select the mixture we need, enter the source data, click the “Calculate” button. (figure 3). To edit the Directories, press select the “Directories” tab (figure 3).
Figure 3. The main window with the connected database.

After clicking the calculate button, a window appears with the main calculation results. To display the calculation in Word, click “Display calculation in Microsoft Word” (figure 4)

Figure 4. The window for displaying the main calculation parameters.

5. Conclusion
As a result of the work, a software tool was designed and developed to automate the calculation of continuous columns.

The software implements the functions of technological calculations: performing the calculation of the necessary concentrations of the initial mixture, distillate and bottom residue; determination of the material balance of the rectification process; calculation of the reflux ratio; determination of volumetric
flow rate of steam; calculation of the diameter of the column; Column height calculation hydraulic
calculation of the column; thermal calculation of the column; calculation of thermal insulation of the
column.

The calculation is made according to a number of standard formulas. These formulas include a large
number of different parameters and reference data.

The advantages of this system are:

- easy to use;
- clarity of data presentation;
- the possibility of additional calculations;
- the possibility to verify data.

The constant automated calculation process will allow the technologist to increase the speed of
completing repetitive tasks and improve the quality of work.

In the future, it is planned to develop a mobile version.

References
[1] Braude E J 2004 Software Engineering Technology p 682
[2] Gorbachev I V 2005 CASE-technology for modeling processes using BPWin and ERWin p 156
[3] Glushakov S V 2002 Databases (St. Petersburg: AST Publishing House) p 504
[4] Zubareva N M 2005 Informatics in Chemistry: Part 2. PASCAL programming language: a
training manual for the study of the discipline "Informatics" and the execution of
computational and graphic work for students of specialties 251100, 320700, 250600, 250100
of all forms of training (Krasnoyarsk: SibGTU) p 157
[5] Mark D A 1993 Methodology of structural analysis and design (Moscow: Metatechnology) p 296
[6] Orlov S A 2012 Software development technology. Modern course in software engineering (St.
Petersburg: Peter) p 608
[7] Pavlov K F 2006 Examples and tasks on the course of processes and apparatuses of chemical
technologies: Textbook for universities (Moscow: LLC TID Alliance) p 576
[8] Chentsova L I 2004 Mass transfer processes A manual on the course "Processes and devices of
chemical production Part 2 (Krasnoyarsk: SibGTU) p 237