Building of a Computer Model for a Complex Distillation Column with Different Locations of Internal Walls

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***Abstract*— Presently one of the major directions in the development of energy-effective distillation processes is the implementation of complex columns with a dividing wall. Despite of active research the usage of such columns is minimal. The reason being the absence of design experience and the control complexity related to the high sensitivity even to minimal disturbances. In this paper, we propose a procedure for preparing a model of a complex column with different positions of internal partitions. The efficiency of the developed procedure is demonstrated by the example of the three-component zeotropic system "ethanol-propanol-butanol" with different feed stream compositions corresponding to different concentration regions.**

Keywords— complex rectifying columns; distillation columns with internal partitions; energy efficiency

Distillation is one of the most energy-consuming processes of separation. At the same time, it is the most widely used industrial method of separation of multicomponent liquid mixtures [1–3].

Currently one of the main directions in the development of energy-effective distillation processes is the implementation of complex columns with a dividing wall (DWC) and complexes with fully or partially coupled thermal and material flows (FTCDS). Leading companies (BASF (Germany), Linde AG (Bavaria), Uhde (Germany), Union Carbide (UOP) USA) are actively develop the dividing wall columns. Annually about five such columns are put into operation [4–13].

The use of such separation options provides up to 20% energy and capital costs savings by reducing the volume of the column and eliminating some of the condensers and boilers.

This causes interest in the creation and study of computer models using simulation programs [14] for mixtures separation in complex dividing wall columns, and determination of optimal operation parameters of these facilities, reducing energy costs as a benefit.

One of the problems with the application of simulation programs is the lack of procedures for calculating complex dividing wall columns. In modern simulation programs, algorithms for calculating distillation columns with several feed and output streams are present [15]. To simulate complex objects, such as stripping sections, column walls, complexes with linked thermal and material flows, the simulation procedure should be a calculation of process flows with a different number of recycle streams. To ensure the calculations convergence of such complexes, it is necessary to develop separate procedures including the selection of optimal algorithms for recycles calculation and physically justified initial approximations. To date, this issue is not sufficiently developed and requires special attention.

In this paper, we propose the procedure for preparing a model of a complex column with different positions of internal walls using the CHEMCAD modeling program.

To demonstrate the procedure for building a computer model of a complex of columns with an internal dividing wall, a column with a centered internal wall was chosen. The initial mixture composition (in mole fractions) "Ethanol (A) 0.1-n-Propanol (B) 0.6-n-Butanol (C) 0.3" and the composition variation range ± 5% of component B in the feed and ± 2% of the variation range in the ratio of components A and C were accepted. The mixture had to be fully divided into individual components, with the purity of each 0.99 mole fraction of the main component.

At the first stage, a model of a complex with a symmetrical sequence of distillation columns was necessary to prepare (Fig. 1), to calculate the material balance under conditions of full separation. Then the material balance of the complex is clarified taking into account the pressure drop in each column and the variations in the initial mixture composition.

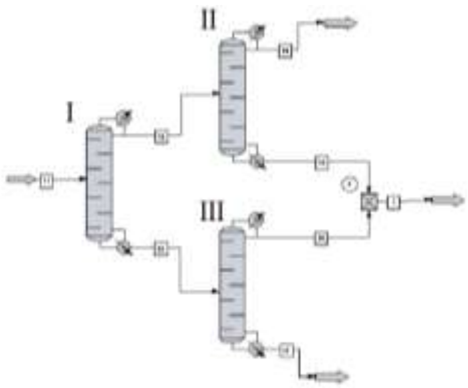

Fig. 1. Complex with a symmetrical sequence of distillation columns

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Since when the columns are combined in a complex column, the middle component is removed as a liquid, it is necessary to equalize the flow rates of the vapor phase returned to the second column from the boiler and the flow of liquid phase returned to the third column from the reflux condenser. It should be remembered that for the first column the type of the condenser must be "partial", as in the simulation of a column with a wall, the first column will turn into a section of a complex column with vapor flowing from its top.

After the material balance calculation, column heights are optimized with regard to the variation in the composition of the feed stream. The resulting column heights are formed by combining the maximum number of trays in rectifying and exhausting sections, to ensure the necessary products purity when of the feed stream composition fluctuates.

Further, for the resulting complex with optimal heights, the material balance is again adjusted to equalize the vapor and liquid flows of the second column boiler and the third column condenser respectively.

In the second stage, the pressure of the top and bottom is calculated for the second and third columns of the complex (Fig. 1), proceeding from the planned number of contact devices and considering the consolidation of the columns into one (i.e. the pressure at the top of column III should equal the pressure at the bottom of column II). At the same time, the height of the first column is increased so that it is equal to the sum of the heights of the exhausting part of column II (below the feeding point) and the rectifying part of column III (the upper part of the column). The feed stage of column I varies in proportion to the height of this column.

At the third stage, the reflux condenser and the boiler of the first column are eliminated, lateral drains from the second and third columns and additional feed streams fed to the first and last trays of the first column are added (Fig. 2). The recycle streams are left open. The parameters of the upper and lower feed flows are equivalent to the parameters of the flow from the first plate of the first column in liquid form and the flow leaving the last plate as a vapor.

After the first column has been calculated and the feed flows for the second and third columns have changed, the reflux ratio of the second column is recalculated on the basis of the simplifying assumption that all excess feed should be condensed and the amount of heat supplied to the boiler of the third column is calculated based on the simplifying assumption that all additional liquid feed needs to be evaporated.

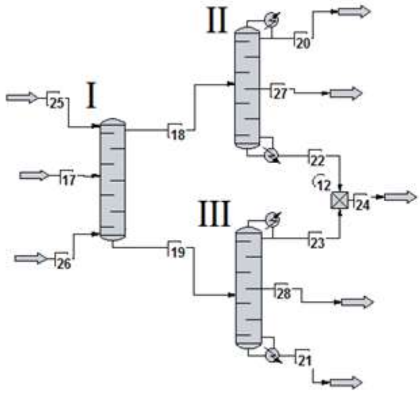

Fig. 2. The computational model of a complex column with a wall on the third stage of the procedure.

At the fourth stage, the recycle streams between the first and second columns are closed, as well as between the first and third columns (Fig. 3). Naturally, having made sure beforehand that the values of the corresponding lateral drains and feed flows equals quite good (the less than 1%difference can be considered satisfactory).

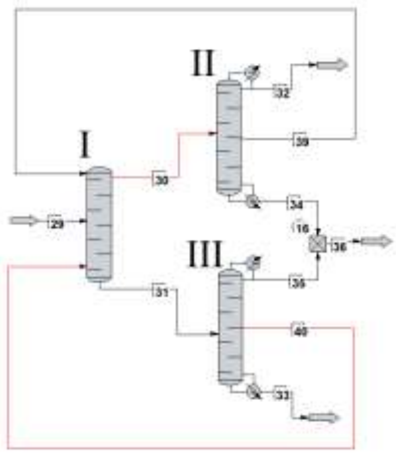

Fig. 3. The computational model of a complex column with a wall on the fourth stage of the procedure.

At the fifth stage, the recycle streams between the second and third columns are closed (Fig. 4), removing the corresponding boiler and reflux condenser. The product stream in the new scheme is formed not as a result of mixing the distillate of the third column and the bottom liquid of the second, but as a lateral drain from the liquid stream flowing from the bottom tray of the second column to the first tray of the third column.

To perform the calculation, initial flow approximations are specified explicitly. Mixing the vapor flow returned to the second column from the boiler and the vapor flow entering the reflux condenser of the third column, the initial approximations for the vapor flow from the top of the third column to the bottom of the second are obtained (Fig. 4). In this case, we proceed from the simplifying assumption that all the vapors of the third column, which had previously entered the boiler, now must pass the entire second column in the form of vapor, condense in the boiler, pass again through the second column in the form of a liquid, and only then separate into side drain and third column reflux.

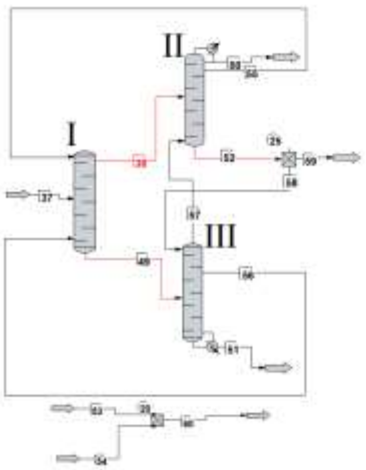

Fig. 4. The computational model of a complex column with a wall on the fifth stage of the procedure.

At the first iteration, product flows and lateral drains are also specified explicitly, then the specifications change according to the required purity of separated products.

It should be noted that this stage is the easiest in the scheme preparation, but the most difficult in terms of convergence.

At the last stage sixth, a new ratio of lateral drain to liquid (for the second column) or vapor (for the third column) leaving the feeding plate (if necessary) is determined for each column. Until now, the formation of flows with specified values for the content of the basic substance for the light and heavy component of the initial mixture was achieved by using the capabilities of the column calculation module. For a lateral drain, theoretically, it would be possible to use a controller (CONT module), in which we would adjust the amount of lateral drain so that the content of the middle component would be equal to a set value. However, in practice for a complex column this cannot be done since it is impossible to uniquely determine the order of the drain change (increase or decrease) when the concentration of the target component deviates from the set value. Depending on whether the light component falls through the middle of the column or if the cube is lifted from the bottom, the direction of correcting the amount of lateral drain will change.

Using a combination of three controllers (two straight and one with back calculation) and two dummy streams (the amount of the average component (kmol / h) in the distillate of the second column and the amount of the average component (kmol / h) in the bottoms of the third column) we get a fictitious stream in which the amount of the average component is equal to the total losses of this substance with light and heavy components released as pure products (Fig. 5). To this fictitious stream, the CONT module (reverse calculation) is installed, on which the amount of side drain will change until it becomes equal to the specified value. A specified value can be defined as the difference between the initial amount of the average component and its losses with the distillate and the bottoms liquid leaving the process flow.

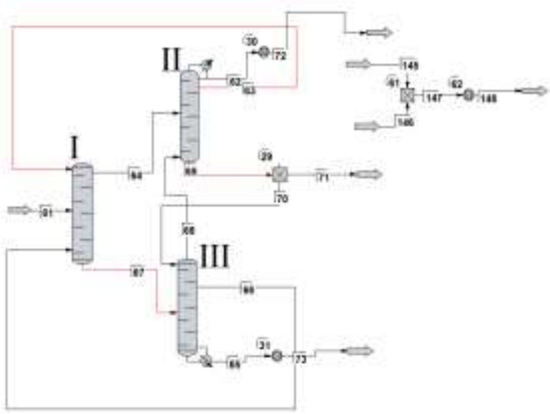

Fig. 5. The computational model of a complex column with a wall on the sixth stage of the procedure.

At this stage the preparing a complex column with a dividing wall in the center can be considered complete, although if desired, it is possible to optimize the columns (height, feeding plate, division of liquid and vapor streams in the lateral drains of the second and third columns). But we must bear in mind that optimization should be done taking into account the purity of the final products with possible fluctuations in the feed composition.

When preparing complex columns with an upper and lower separation wall, it is necessary to use the same principles as for a complex column with a centered wall.

The efficiency of the described procedure for modeling of complex columns with the upper, lower and central internal walls is demonstrated using the example of the three-component zeotropic system "ethanol-propanol-butanol" for six feed stream compositions corresponding to different concentration regions:

Composition	**Ethanol**	**Propanol**	**Butanol**
1	0.50	0.20	0.30
2	0.10	0.20	0.70
3	0.10	0.60	0.30
4	0.30	0.30	0.40
5	0.22	0.58	0.20
6	0.15	0.35	0.50

Table 1 shows the obtained values of the total thermal loads of complex columns with different positions of internal walls with different compositions of the feed stream.

TABLE I. TOTAL THERMAL LOADS OF COMPLEX COLUMNS WITH VARIOUS POSITION OF INTERNAL WALLS AT DIFFERENT COMPOSITIONS OF THE FEED STREAM.

Composition	**Total thermal load of the complex, kcal / h**		
	A complex column with an upper wall	A complex column with a lower wall	A complex column with a central wall
1	**137.94**	139.00	146.11
2	122.51	**104.47**	129.65
3	171.21	173.26	**119.07**
4	**141.39**	184.66	152.69
5	167.56	171.39	**139.28**
6	144.29	**133.99**	136.79

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