

# Development Of The Mathematical Model And Automated Functional-Technological Scheme Of The Rectification Process

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**Annotatsiya.** This article presents the development of a mathematical model of the rectification process and proposes an automated functional-technological scheme for effective process control. During the research, the heat and mass transfer processes occurring in the rectification column were analyzed, and their mathematical expressions were derived. Based on the developed model, the factors affecting the main process parameters were identified and their interrelationships were studied. In addition, a functional-technological scheme for designing an automated control system was developed, in which measurement, monitoring, and control devices were integrated. The proposed approach makes it possible to improve the stability of the rectification process, reduce energy consumption, and enhance product quality.

**Keywords:** Mathematical model, distillation, volatile component, functional-technological scheme, equilibrium diagram, material balance.

A rectification unit is a chemical-technological device designed to separate liquid mixtures into fractions (distillation). Complete separation of solutions is mainly carried out by the rectification method. This process is usually performed in packed or tray columns and makes it possible to obtain components in separate compositions by effectively utilizing the differences in their boiling points.

In the column, vapor and liquid move in opposite directions. In each contact zone, part of the vapor condenses, while the liquid partially evaporates due to the heat released during condensation. This process ensures efficient separation of the components based on their evaporation and condensation characteristics.

As a result, the vapor phase in the column becomes enriched with more volatile components, whereas the liquid phase becomes enriched with less volatile components. This phenomenon, which is based on the evaporation properties of the components, increases the efficiency of the rectification process and enables a high degree of separation of the mixture components.

As a result of repeated mass exchange between the vapor and the liquid, the distillate mainly consists of highly volatile components, while the bottom residue in the column becomes enriched with less volatile components.

The following basic assumptions are accepted in the modeling and calculation of the rectification process:

➤ According to this assumption, during the condensation of 1 kmol of vapor, 1 kmol of liquid evaporates. This ensures that the vapor flow rate remains constant throughout any cross-sectional area of the rectification column.

➤ It is assumed that the composition of the vapor condensing in the dephlegmator remains constant. According to this assumption, the composition of the vapor leaving the rectification column is equal to the composition of the distillate.

When the initial solution with concentration  $x_1$  is heated to the boiling temperature  $t_1$ , thermodynamic equilibrium is established between the liquid and vapor phases. During this process, when the generated vapor is condensed, a liquid enriched with the more volatile component and having a concentration equal to  $x$  is obtained (Figure 1).

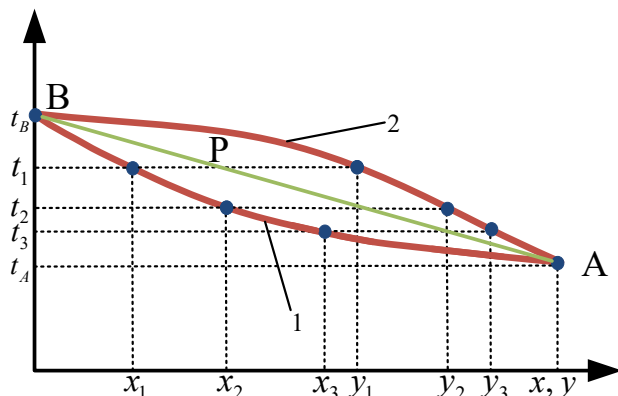


Figure 1. «t - x - y» equilibrium diagram at P= const (constant pressure):1- boiling curve of the liquid phase, 2- condensation curve of the vapor phase.

The «t - x - y» equilibrium diagram at P = const (constant pressure) is a graphical representation that describes the thermodynamic relationship between temperature and the compositions of the liquid and vapor phases for a binary (two-component) system.

### Material and Methods

This diagram plays an important role in the analysis of rectification and distillation processes, as it makes it possible to determine the boiling temperature of the liquid for each composition and the composition of the vapor at that temperature.

#### The main elements of the diagram, i.e., the axes:

- On the horizontal axis, the composition of the liquid phase of the mixture  $x$  (in mole fraction) is plotted.;
- On the vertical axis, temperature  $t$  ( $^{\circ}\text{C}$ ) is plotted;
- The vapor phase composition  $y$  is also represented on the same axis as  $x$ , and the equilibrium points between the two phases are shown.

If the liquid is further heated until its temperature reaches  $t_2$ , the vapor formed, when condensed, produces a liquid with composition  $x_2$ . In this way, when the processes of evaporation and condensation are repeated several times, it becomes possible to separate the initial solution into its components, namely the more volatile and less volatile components, in a purer form.

In chemical technologies, various mass transfer mechanisms are widely used in separation and purification processes. These processes include absorption, extraction, rectification, adsorption, and drying. In absorption, gaseous or vapor-phase substances are transferred into a liquid phase, while in extraction, components are distributed between two or more liquid phases. Rectification ensures separation based on boiling point differences and phase equilibrium. In adsorption, substances are taken up on large surface areas, whereas drying removes moisture from materials to increase their concentration. These processes enable control over the distribution of components between phases in chemical-technological systems and improve product quality to an optimal level. At the same time, the rectification process is governed by molecular diffusion, mass transfer, and thermodynamic equilibrium principles.

Although these processes differ in nature and implementation within technical equipment, they all follow common fundamental laws. Therefore, mass transfer processes such as rectification, absorption, extraction, and adsorption share certain common features as automation objects. In these systems, similar

methods are used for monitoring, controlling, and optimizing process parameters. These common characteristics are essential for mathematical modeling of processes, designing controllers, and developing control systems.

Figure 2 illustrates a schematic representation of the general operating principle of a rectification column.

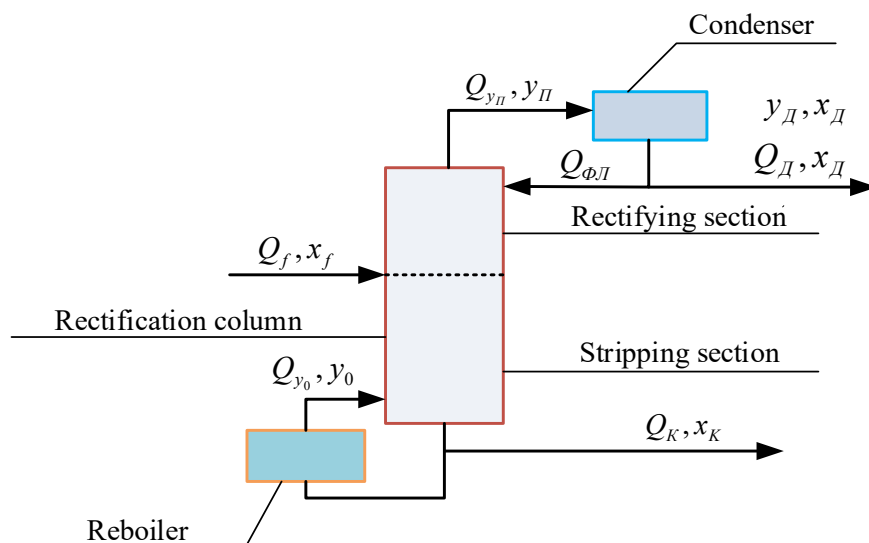


Figure 2. Schematic representation of the general operating principle of a rectification column.

According to this scheme, the scientifically based theoretical description of the process is as follows: the initial solution  $Q_f, C_f$  (the flow rate of the mixture entering the column and its molecular or molar composition) is heated to a specified temperature and fed into the middle section of the column.

At the bottom of the column, the liquid is heated using a reboiler, generating a vapor phase ( $Q_{y_0}, C_{y_0}$ ). The formed vapor rises upward and comes into contact with the liquid flowing downward from the top. During each contact (mass transfer stage), part of the vapor condenses, while the liquid partially evaporates due to the heat released during condensation.

In the upper enriching section of the column, the liquid phase flows downward while the vapor phase moves upward. As a result of this counter-current flow, heat and mass transfer occur between the phases. Consequently, the vapor phase becomes enriched with the more volatile component, whereas the liquid phase becomes enriched in the less volatile component.

This vapor ( $Q_p, C_p$ ) is passed through a dephlegmator (condenser), where it is converted into liquid. A portion of the resulting condensate is returned to the column as reflux ( $Q_{FL}$ ), while the remaining part is withdrawn as distillate ( $Q_D, C_D$ ).

The residual liquid at the bottom of the column is withdrawn as the bottom product ( $Q_K, C_K$ ). This residue is enriched with the less volatile components. In this way, components are separated along the height of the column according to their volatility.

Therefore, the intensity of heat and mass transfer at each stage along the column is one of the key factors determining the overall efficiency of the process.

In general, the efficient operation of a rectification column depends on the following conditions:

- proper selection of the internal structure of the column (trays, packings);
- optimal control of pressure and temperature ( $P=\text{const}$ );
- maintaining the reflux ratio and reflux flow coefficient at optimal levels;
- ensuring the stability of the heat balance.

## Results

As a result, the rectification process enables the separation of complex liquid mixtures into high-purity component fractions, which are widely used in the chemical, petroleum refining, food, and pharmaceutical industries.

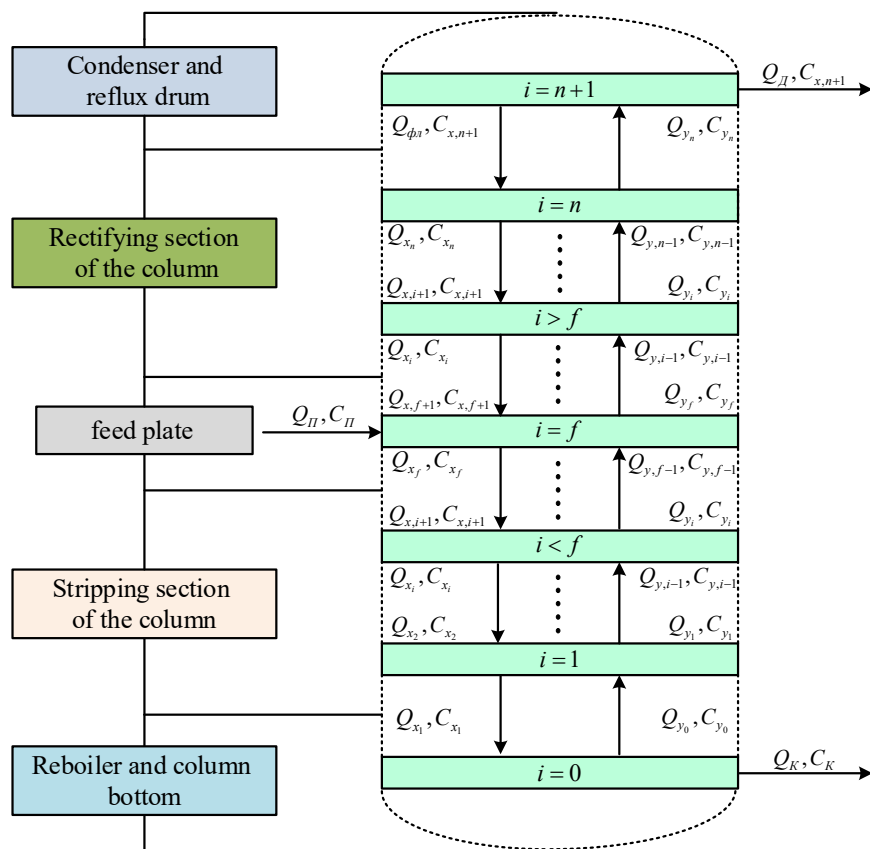


Figure 3. Structural scheme of a rectification unit.

**Mathematical description of the lower part of the rectification column**

The lower part of the rectification column (the reboiler section) is an important element of the process, where evaporation of the liquid phase occurs and the bottom product (residue) is formed. The mathematical model of this section is typically based on mass balance, energy balance, and phase equilibrium equations. The structural scheme illustrating the design of the reboiler and its functional interaction is shown in Figure 4.

The structural scheme of the reboiler and boiler illustrates their design structure, main technological elements, and functional interconnections in a systematic manner. Through this scheme, the supply of thermal energy, the evaporation process, interphase transfer, and changes in process parameters (temperature, pressure, and flow) are clearly and logically represented in a sequential order. The structural scheme serves as an important source of information for mathematical modeling, process automation, and the development of control algorithms.

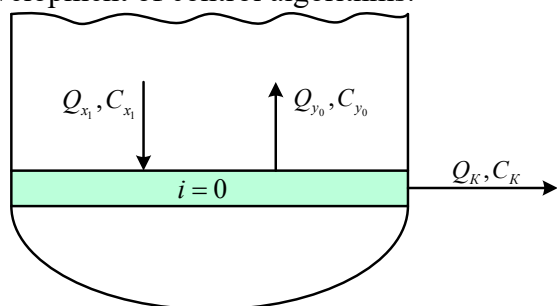


Figure 4. Structural scheme illustrating the configuration of the reboiler and boiler and their mutual functional interaction.

In the region covering the lower part of the column, a heat balance analysis is carried out by taking into account heat fluxes and energy exchange processes.

**The overall mass balance for the bottom section of the column is written as follows:**

$$\frac{dM_b}{dt} = \rho \cdot S \cdot \frac{dh_b}{dt} = Q_{x_1} - Q_{y_0} - Q_K \quad (1)$$

In this case:  $M_b$  – the total mass of the liquid phase accumulated in the bottom (reboiler) section of the column;  $\frac{dM_b}{dt}$  – the rate of change of this mass with respect to time;  $\rho$  – the density of the liquid accumulated in the bottom (reboiler) section of the column [ $kg/m^3$ ];  $S$  – the cross-sectional area of the reboiler (bottom section of the column) [ $m^2$ ];  $h_b$  – the variable liquid level in the reboiler;  $Q_{x_1}$  – the feed flow rate of the initial mixture;  $Q_{y_0}$  – the vapor flow rate generated in the heater (reboiler);  $Q_K$  – the flow rate of the bottom residual liquid, i.e., the reboiler (bottom) product.

This equation is based on the law of conservation of mass and describes the accumulation or depletion of material in the lower part of the column over time. If the process is operated under steady-state conditions, then  $\frac{dM_b}{dt} = 0$ , and the mass balance is determined by the equality of incoming and outgoing flows. In this case, the overall material balance takes the following form:

$$Q_{x_1} = Q_{y_0} + Q_K \quad (2)$$

Based on (1) and (2), the following can be calculated:  $h_b = f(Q_K, Q_{y_0})$ .

The bottom section of the column is the main center of energy and heat transfer processes. In this region, due to the interaction between gas and liquid phases, heat fluxes are generated, which directly affect the efficiency of the column and the quality of the product. Therefore, determining the heat balance of the lower section is of great importance. The heat balance is usually expressed based on the law of conservation of energy by considering incoming and outgoing heat flows.

The component mass balance is determined by accounting for the inflow and outflow of each chemical component in the system, as well as the changes caused by internal processes.

#### Material balance for the separated (more volatile) component.

In the considered system, the material balance equation for the separated more volatile component is formulated by taking into account the input of this component into the system, its output, and its accumulation within the system. This balance is important for evaluating process efficiency and constructing the mathematical model.

In general, the material balance for the more volatile component is expressed as follows:

$$\frac{dM_b C_{x_0}}{dt} = Q_{x_1} C_{x_1} - Q_{y_0} C_{y_0} - Q_K C_{x_0} \quad (2)$$

in this case:  $C_{x_1}$  – the composition of the liquid flowing from the top.,  $C_{y_0}$  – the mole fraction of the component in the vapor phase,  $C_K$  – the concentration of the component in the liquid phase of the bottom product.

If the amount of the incoming component is greater than the outgoing amounts, the more volatile component accumulates in the reboiler. Equation (2) is also based on the law of conservation of mass and describes the input, output, and time-dependent accumulation of the more volatile component in the lower part of the column. If the process is operated under steady-state conditions, then  $\frac{d(M_b C_{x_0})}{dt} = 0$ , there is no accumulation of matter, the component concentrations remain constant over time, and all incoming and outgoing material flows are in equilibrium:

$$Q_{x_1} C_{x_1} = Q_{y_0} C_{y_0} + Q_K C_{x_0}$$

For the purpose of simplifying the mathematical model, it is assumed that the reboiler operates in a complete evaporation regime;  $C_{y_0} = C_{x_0}$  as a result, the component concentrations in the vapor and liquid phases are considered equal.

Based on equations (3) and (4), it can be written as follows:

$$C_K = f(Q_{x_1}, Q_K, Q_{y_0}, C_{x_1})$$

The energy balance process is carried out by comparing the amount of energy entering the system (in the form of heat, work, and other energy forms) with the energy leaving the system. This analysis, based on the law of conservation of energy, makes it possible to determine the changes in energy within the system.

The energy balance for the lower section is expressed as follows:

$$\frac{dM_b \eta_b}{dt} = Q_{x_1} \eta_{x_1} - Q_{y_0} \eta_{y_0} + Q_b$$

in this case:  $\eta_b, \eta_{x_1}$  – the enthalpies of the bottom product and the incoming liquid, respectively;  $\eta_{y_0}$  – the enthalpy of the vapor phase,  $Q_b$  – the heat flow supplied to the reboiler.

### Phase equilibrium equation

Phase equilibrium describes a condition in which multiple phases in a system (for example, vapor and liquid) are in mutual interaction, while their composition and thermodynamic state remain constant over time. Mathematically, this state is described using phase equilibrium equations. The equilibrium condition is defined by the equality of chemical potentials of each component across the phases:

$$\mu_i^{(\text{liquid phase})} = \mu_i^{(\text{vapor phase})}, i = 1, 2, 3, \dots, n,$$

In this case,  $\mu_i^{(\text{liquid phase})}, \mu_i^{(\text{vapor phase})}$  denotes the chemical potentials of component  $i$  in the liquid and vapor phases, respectively. In practical calculations, this equation is often expressed in terms of equilibrium constants or distribution coefficients and is transformed into the following form:

$$y_i = k_i x_i$$

In this case,  $x_i$  and  $y_i$  are the mole fractions of component  $i$  in the liquid and vapor phases, respectively, and  $k_i$  is the equilibrium (distribution) coefficient between the phases. These equations are of great importance in analyzing interphase mass transfer, modeling separation processes, and determining the optimal operating conditions of technological equipment.

### Description of the informational (data-flow) scheme of the lower part of the column

The informational (data-flow) scheme of the lower part of the rectification column describes the functional interconnection between measuring and control instruments and signal transmission channels that ensure the identification, measurement, and processing of the main technological parameters of the process.

The lower part of the column, as a multivariable (multi-connected) object, is represented in the informational scheme organized according to the  $h_k$  or  $h_k, C_k$  principles as an integrated system in which material and energy flows, as well as control and regulation signals, are mutually interconnected. This scheme is modeled based on the functional role of each component, the interaction between input and output flows, and both dynamic and static relationships.

In this way, the information model of the lower section of the column enables process parameter optimization, ensures stable system operation, and allows analysis of system responses under various operating conditions.

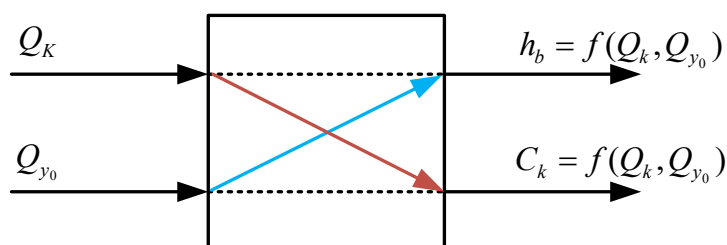


Figure 5. Information scheme of the lower part of the column as a multi-input multi-output object with parameters  $h_b$  or  $h_k$  and  $C_k$ .

To simplify the discussion, let us consider only two channels; then a more detailed scheme can be represented as shown in Fig. 6. Here,  $y_1$  and  $y_2$  are control signals, while  $x_1^{out}(t)$  and  $x_2^{out}(t)$  are the actual values of the controlled variables.

In a well-designed system, the channels  $y_1(t) \rightarrow x_1^{in}(t)$  and  $y_2(t) \rightarrow x_2^{in}(t)$  are independent, i.e., the output  $x_1^{in}(t)$  is controlled only by the signal  $y_1(t)$ , and  $x_2^{in}(t)$  is controlled only by the signal  $y_2(t)$ . In other words, the signal  $y_1(t)$  does not influence  $x_2^{in}(t)$ , and  $y_2(t)$  does not affect  $x_1^{in}(t)$ .

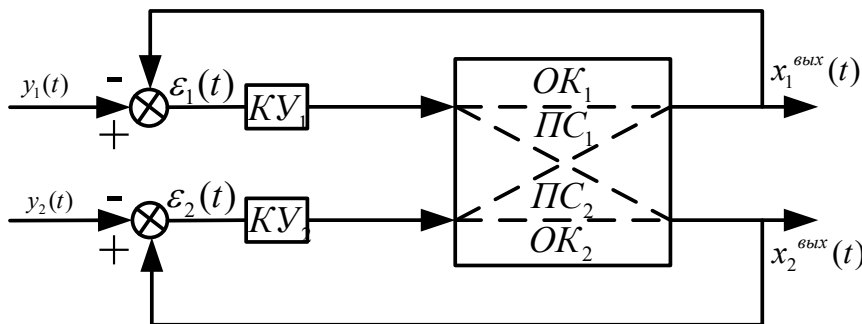


Fig. 6. Structural scheme of a two-dimensional system.

In real systems (along with the main channels  $OK_1$  and  $OK_2$ ), cross-couplings are often present:  $PC_1$  (the signal  $y_1(t)$  affects the output  $x_2^{out}(t)$ ) and  $PC_2$  (the signal  $y_2(t)$  affects the output  $x_1^{out}(t)$ ).

When studying such systems, as well as when designing controllers (corrective devices  $KV_1$  and  $KV_2$ ), it is necessary to take into account the cross-couplings  $PC_1$  and  $PC_2$ . The system is called autonomous if, due to imposed additional connections, the mutual influence of channels is eliminated (i.e.,  $PC_1$  and  $PC_2$  are absent).

The general characteristic of mass transfer processes is their high energy capacity, and the main goal of automation is to reduce energy consumption while maintaining product quality at a specified level.

Almost all mass transfer processes are carried out in column-type apparatuses with a diameter of several meters and a height of several tens of meters. Therefore, their dynamic characteristics are characterized by a large time constant and significant delay. Under such conditions, single-loop simple control systems lead to large dynamic errors and long transient responses. In order to improve the quality of transient behavior in control systems, combined and cascade automatic control systems are widely used in mass transfer processes.

### Discussion

One of the main difficulties in automating mass transfer processes is the absence of continuous automatic analyzers for monitoring product composition. In such cases, composition control is performed indirectly through parameters such as boiling temperature of the mixture or its density. However, these control systems introduce additional complexity, as they require determining the relationship between composition and indirect parameters while also accounting for the influence of disturbance factors.

Rectification units are used for separating liquid homogeneous mixtures into individual components or groups of components through the counter-current interaction of vapor and liquid mixtures.

The automation object of a rectification unit is considered using the example of a binary mixture containing a light volatile component  $C_D, C_K$ , where separation is carried out into distillate (a liquid formed from purified vapor) and a bottom product enriched with light volatile components  $C_D$  and  $C_K$ .

We accept the following notations (see Fig. 7):  $Q_T, Q_D, Q_K, Q_B, Q_{I.T}, Q_{s.a}, Q_{FL}$  - maintenance costs; distillate; bottom (residue) product; heating steam for boiling; heat carrier for heating the supply source; cooling agent (in the dephlegmator); liquid agent; reflux;  $r_b$  - enthalpy of heating steam;  $\theta_{I.T}, \theta_{s.a}$  - temperatures of the heat carrier and cooling agent;  $C_{I.T}, C_{s.a}$  - specific heat capacities of the heat carrier and cooling agent;  $P_K$  - pressure in the column;  $h_K, h_{FL}$  - liquid levels in the column bottom and reflux drum.

The rectification unit is a complex object with a large number of interrelated coordinated parameters. Therefore, to properly analyze its static and dynamic characteristics, it is necessary to perform a thorough study of the object. In such analysis, the main controlled (output) coordinates of the object are considered to

be the concentrations of distillate and bottom product  $C_D, C_K$ , the liquid level in the column bottom  $h_K$ , the level in the reflux drum  $h_{FL}$ , and the column pressure  $P_K$ .

The manipulated (input) variables in the rectification column include the heating steam flow rate  $Q_B$ , heat carrier flow rate  $Q_{I.T}$ , cooling agent flow rate  $Q_{s.a}$ , distillate outlet flow rate  $Q_D$ , bottoms product flow rate  $Q_K$ , and reflux flow rate  $Q_{FL}$ .

Since the feed mixture is supplied to the rectification column from other technological units, variations in its flow rate, composition, and temperature are considered the main disturbance factors in the process. In addition, disturbances also include the enthalpies of the heating steam, heat carrier, and cooling agent, as well as heat losses to the environment  $q$ .

In practice, among these disturbances, only the feed temperature  $t$  is regulated, while the feed flow rate  $Q_T$  is monitored. The feed composition is rarely controlled, whereas the remaining disturbance factors are generally not directly measured or regulated.

Taking the above into account, the automated functional-technological scheme of the rectification process is presented in Figure 7.

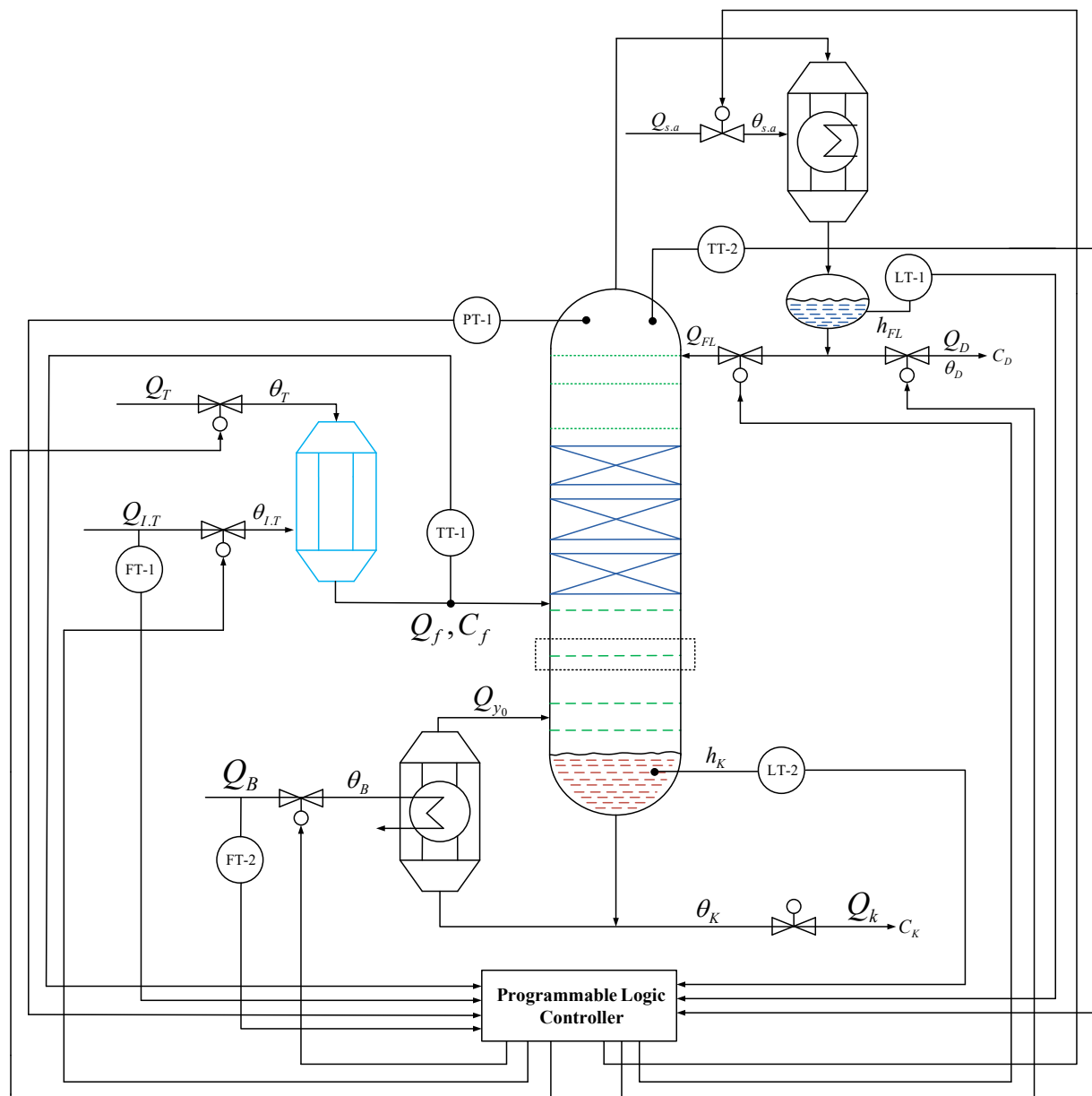


Figure 7. Automated functional-technological scheme of the rectification process.

**Conclusion.** As a result of the study, a mathematical model of the rectification process was developed and the factors affecting its main parameters were identified. The proposed model enables in-depth analysis of the process and the development of optimal control strategies. In addition, an automated functional-technological scheme was designed, which ensures real-time monitoring and control of the process.

As a result, the reliability and efficiency of the system are improved, dependence on human factors is reduced, and rational use of energy resources is achieved. In the future, the process can be further improved by applying modern control methods (such as adaptive and predictive control) based on the developed model and scheme.

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