A prerequisite for the research is the potential for the design of high-precision automated control systems (ACS) of almost any complexity using advanced digital equipment.

Urgent problem is the actual application of such systems in industrial automation. Complex precise systems virtually exclude the adjustment stage from the start-up process. So, ACS should be modeled as accurately as possible before being put to use. This means that the synthesis and modeling of precise ACS shall consider:
- non-linearity of the behavior of a real process;
- hydrodynamic operating conditions of controllers;
- properties of actuators;
- errors and dynamics of the chosen sensors.

This ensures the behavior proximity of ACS in modeling and in real operation conditions.

The urgency of the design of a precise ACS of a vitamin B6 synthesis reactor is caused by the fact that vitamin B6 is a valuable substance for the pharmaceutical, food and agricultural industries. Although vitamin B6 can be produced in many ways, its long-term industrial production is based on chemical synthesis. The production process is completed by nitrination of pyridone, fed as a suspension with acetic anhydride into a jacketed continuous stirred-tank reactor. The pharmaceutical industry requires a stable vitamin with minimum impurities. Stable composition, purity and prevention of potential process danger caused by the rate and exothermic nature of the reaction, are ensured by the precise ACS.

The literature review [1] shows that, despite a possibility of designing ACS of any complexity and quality, simple systems based on PID controllers prevail (up to 90%) in the world industrial automation. At the same time, the precise control problem is paid attention to in the development of weapons [2], electric drives [3], robotics [4], precise mechanics [5]. In general, few works are available regarding the problem of precise control in industrial automation. The main reason is the established practice of simplified modeling of the control object and neglect of the control equipment properties.

One of the objects that require precise control is a pharmaceutical chemical reactor. For the design of high-precision ACS, modeling of the reactor is performed in the class of nonlinear lumped-parameter systems. Such modeling has been considered, for example, in the fundamental paper [6]. The number of the reactor equations depends both on the chemical conversions occurring in the reactor, and on the presence of thermodynamic reaction effects. This can be two equations for direct feedstock conversion into a product [7], or a chain of more equations for multistage feedstock conversion in view of thermodynamics [8]. The nonlinear model of a chemical reactor is sometimes considered as a family of linear models [9].

As a rule, adjustable parameters in the reactor are concentration of the final product, temperature and product level [6] that is neglected in simple cases. In addition to conventional PID controllers, neural networks and other artificial intelligence methods [10, 11], adaptive [9] and oth-
er types of controllers are also used. However, the designed ACS is not responsive to the properties of the control equipment operating in the system.

The literature on the control equipment considers the models of controllers, taking into account, for example, the geometry of valves [12], correlation between the controller friction and speed [13], etc. At the same time, modeling of such equipment and measuring system errors in combination with a dynamic model of an industrial plant has been hardly examined.

Among the pharmaceutical reactors, the focus of research is the vitamin B₆ synthesis reactor. Vitamin B₆ is a valuable substance for the pharmaceutical, food and agricultural industries. Although vitamin B₆ can be produced in many ways, its long-term industrial production is based on chemical synthesis [14]. The production process is completed by nitration of pyridone, fed as a suspension with acetic anhydride into a jacketed continuous stirred-tank reactor. The pharmaceutical industry requires a stable vitamin with minimum impurities.

Thus, development of an approach to the synthesis and modeling of precise ACS, in particular, of the vitamin B₆ synthesis reactor, is a challenge.

3. Goals and objectives

The goal of the research is to develop an approach to the design of precise control systems of nonlinear objects. Based on the proposed approach, a modern precise control system of a reactor in the production of vitamin B₆ is developed.

In order to achieve the goal, the following objectives need to be accomplished:
– to develop a mathematical model of the dynamics of the control object;
– to develop a model of the variation of the hydraulic friction coefficient;
– to develop a model of the controller and automation equipment;
– to develop a precise ACS of the vitamin B₆ synthesis reactor.

4. Methods of research of objectives accomplishment in the design of precise control systems of nonlinear objects

A brief description of the research methods used to accomplish the objectives is given in Table 1.

The research was conducted with the help of the Matlab software system, including the Toolboxes Control System and System Identification. The resulting controller can be implemented in a real-time system using the Matlab Coder tool.

The design quality criterion is formed as a result of accurate modeling of the developed control system, which involved all the models obtained by accomplishing the objectives 1–5.

The transients resulting from the modeling should give small deviations in concentration (±6 mol/m³), temperature (±1 °C) and level (±20 mm) of a product in the reactor under significant flow rate disturbances.

Small deviations in concentration ensure a high quality of vitamin B₆, small deviations in temperature and level of a product provide the process safety in the reactor.

5. Results of objectives accomplishment in the design of precise control systems of nonlinear objects

5.1. Development of an analytical nonlinear mathematical model of the dynamics of a control object

In terms of modeling, the vitamin B₆ synthesis reactor is an ideal stirred-tank reactor, which receives flows of concentrated nitric acid and a suspension of pyridone with acetic anhydride. The reaction of pyridone with acid is exothermic, so the reactor includes a mixture cooling jacket. Nitration is a first-order reaction [14].

The mathematical model of the reactor is based on the standard equations of chemical kinetics and thermodynamics of chemical reactions [17]. The model has the following form

\[
\frac{dx}{dt} = \left( u_1 \cdot \rho_1 + u_2 \cdot \rho_2 - k_3 \cdot \sqrt{x_1 \cdot \rho / S} \right) / \rho,
\]

\[
\frac{d(x_1 \cdot x_2)}{dt} = \frac{u_1 \cdot C_1 + u_2 \cdot C_2 - k_3 \cdot \sqrt{x_1 / S \cdot x_2}}{1 + k \cdot e^{(R/T \cdot x_1 \cdot S)}} \cdot x_2,
\]

\[
\frac{d(x_1 \cdot x_3)}{dt} = \frac{u_1 \cdot C_1 \cdot \rho_1 \cdot T_1 + u_2 \cdot C_2 \cdot \rho_2 \cdot T_2 - k_3 \cdot \sqrt{x_1 / S}}{1 + k \cdot e^{(R/T \cdot x_1 \cdot S)} \cdot x_3} \cdot H - c_1 \cdot u_1 \cdot \rho_1 \cdot (x_1 - x_3) + \frac{c \cdot \rho}{c_1 \cdot \rho} \cdot (c_1 \cdot u_1 \cdot \rho_1 \cdot (T_1 - x_1) + S \cdot k \cdot (x_1 - x_3)) / (c_1 \cdot V \cdot \rho).
\]

Table 1

<table>
<thead>
<tr>
<th>Objective</th>
<th>Research method</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Analytical development of a nonlinear model of dynamics of the vitamin B₆ synthesis reactor. Using the laws of mass action and chemical thermodynamics, the model is developed as a system of nonlinear differential equations. The order of the equations is defined by the order of the reaction occurring in a chemical reactor.</td>
</tr>
<tr>
<td>2</td>
<td>Approximation of the Colebrook-White nomogram. The research consists in considering the variation of the hydraulic friction coefficient (λ) with the fluid velocity. The variation of λ is caused by the nature of the control process, which involves different amounts of the control flow depending on the controller opening rate.</td>
</tr>
<tr>
<td>3</td>
<td>Analytical compilation of a model of the combined effect of the valve on the fluid flow in a pipeline, taking into account the flow velocity and λ, the linear or equal percentage flow characteristic of the valve.</td>
</tr>
<tr>
<td>4</td>
<td>Development of an analytical model of automation equipment, taking into account its characteristics, errors and dynamics. Dynamics is usually considered as the first-order, possibly delay, differential equation.</td>
</tr>
<tr>
<td>5</td>
<td>Analytical design of optimal multivariable controllers for the design of a precise control system of the vitamin B₆ synthesis reactor</td>
</tr>
</tbody>
</table>


The designations and nominal values of the model parameters are given in Table 2. The variables whose regime values are to be set are designated separately. These variables are \( y_i = x_i \), \( i = 1, 2, 3 \).

### Table 2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Specification</th>
<th>Nominal value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( u_1 )</td>
<td>nitric acid flow rate</td>
<td>0.0918</td>
<td>m³/s</td>
</tr>
<tr>
<td>( u_2 )</td>
<td>pyridone suspension flow rate</td>
<td>0.0106</td>
<td>m³/s</td>
</tr>
<tr>
<td>( u_3 )</td>
<td>cooling water flow rate</td>
<td>0.012</td>
<td>m³/s</td>
</tr>
<tr>
<td>( x_1 )</td>
<td>reactor mixture volume</td>
<td>4.8</td>
<td>m³</td>
</tr>
<tr>
<td>( x_2 )</td>
<td>( B_0 ) molar concentration</td>
<td>0.132</td>
<td>kmol/m³</td>
</tr>
<tr>
<td>( x_3 )</td>
<td>( B_0 ) temperature</td>
<td>41</td>
<td>kmol/m³</td>
</tr>
<tr>
<td>( x_4 )</td>
<td>jacket water temperature</td>
<td>15</td>
<td>°C</td>
</tr>
<tr>
<td>( F )</td>
<td>( B_0 ) flow rate</td>
<td>0.0152</td>
<td>m³/s</td>
</tr>
<tr>
<td>( C_1 )</td>
<td>HNO₃ molar concentration</td>
<td>0.61</td>
<td>kmol/m³</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>pyridone molar concentration</td>
<td>0.129</td>
<td>kmol/m³</td>
</tr>
<tr>
<td>( T_1 )</td>
<td>HNO₃ temperature</td>
<td>20</td>
<td>°C</td>
</tr>
<tr>
<td>( T_2 )</td>
<td>pyridone suspension temperature</td>
<td>41</td>
<td>°C</td>
</tr>
<tr>
<td>( k )</td>
<td>rate constant</td>
<td>1.6×10¹¹</td>
<td>s⁻¹</td>
</tr>
<tr>
<td>( E )</td>
<td>activation energy</td>
<td>83.25</td>
<td>kJ/mol</td>
</tr>
<tr>
<td>( R )</td>
<td>universal gas constant</td>
<td>8.31</td>
<td>J/(mol·°C)</td>
</tr>
<tr>
<td>( n )</td>
<td>order of reaction</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>( H )</td>
<td>thermal effect of nitration</td>
<td>1.3×10³</td>
<td>J/(mol·°C)</td>
</tr>
<tr>
<td>( c )</td>
<td>( B_0 ) heat capacity</td>
<td>1.550</td>
<td>J/(kg·°C)</td>
</tr>
<tr>
<td>( \rho )</td>
<td>( B_0 ) density</td>
<td>1.431</td>
<td>kg/m³</td>
</tr>
<tr>
<td>( c_1 )</td>
<td>HNO₃ heat capacity</td>
<td>1.744</td>
<td>J/(kg·°C)</td>
</tr>
<tr>
<td>( \rho_1 )</td>
<td>HNO₃ density</td>
<td>1.400</td>
<td>kg/m³</td>
</tr>
<tr>
<td>( c_2 )</td>
<td>pyridone suspension heat capacity</td>
<td>1.529</td>
<td>J/(kg·°C)</td>
</tr>
<tr>
<td>( \rho_2 )</td>
<td>pyridone suspension density</td>
<td>1.696</td>
<td>kg/m³</td>
</tr>
<tr>
<td>( S )</td>
<td>heat transfer area</td>
<td>14.6</td>
<td>m²</td>
</tr>
<tr>
<td>( k_1 )</td>
<td>coefficient of heat transfer to water</td>
<td>947</td>
<td>W/(m²·°C)</td>
</tr>
<tr>
<td>( V_w )</td>
<td>jacket water volume</td>
<td>0.585</td>
<td>m³</td>
</tr>
<tr>
<td>( c_w )</td>
<td>jacket water heat capacity</td>
<td>4.179</td>
<td>J/(kg·°C)</td>
</tr>
<tr>
<td>( \rho_w )</td>
<td>jacket water density</td>
<td>992.1</td>
<td>kg/m³</td>
</tr>
<tr>
<td>( T_w )</td>
<td>inlet water temperature</td>
<td>8</td>
<td>°C</td>
</tr>
</tbody>
</table>

Let’s standardize the model. To do this, we introduce the column vector \( g \), containing the right members of DE of the system (1), and the matrix \( A \), belonging to the DE left member. Then we get the model in the following form

\[
\frac{dx}{dt} = A^{-1} \cdot g,
\]

where

\[
g = \begin{bmatrix} g_1 & g_2 & g_3 & g_4 \end{bmatrix},
\]

\[
A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ x_2 & x_1 & 0 & 0 \\ x_3 & 0 & x_1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.
\]

Thus, the analytical nonlinear mathematical model of the dynamics of a control object has been developed.

### 5. 2. Development of a model of variation of the hydraulic friction coefficient

For calculation of hydraulic friction \( \lambda \) in round pipes under the flow rate variation, and, therefore, the Reynolds number, a special procedure was developed. It uses the current Reynolds number value (Re), and also the ratio of the pipeline inner diameter to the equivalent pipe roughness \( (n, = D/\Delta_n) \) as input parameters. The procedure body is an approximation of the well-known Colebrook-White nomogram for determining the coefficient of hydraulic friction \( \lambda \), as well as the Stokes equation and approximation of the transient regime.

The developed model has the following form

\[
\lambda = A + K \cdot \left(1 - e^{-\frac{\lg(n)}{t}}\right),
\]

\[
t = \lg(Re),
\]

\[
x = \lg(n),
\]

where the coefficients of equation (4) are determined by the relationships (5)–(7)

\[
T = 1.14 \cdot 10^{15} \cdot e^{-\frac{(x-5.5)^3}{15}} - 0.29 \cdot e^{\frac{(x-2.4)^3}{23}} + 1.13 \cdot e^{-\frac{(x-4.6)^3}{50}},
\]

\[
A = \frac{1.91 \cdot 10^{-1} \cdot x^{-5.2} + 39}{1000},
\]

\[
K = \frac{184.2 \cdot x^{-2.6} - 131.7}{1000}.
\]

The result of modeling for the function

\[
\lambda = f\left(\text{Re}, D/\Delta_n\right)
\]

is shown in Fig. 1 and corresponds to the Colebrook-White nomogram [18].
The modeling revealed the difference of the linear and equal percentage flow characteristics of valves constructed using the variable $\lambda$ from characteristics constructed using the averaged value $\bar{\lambda}$. The variable $\lambda$ was calculated from the approximation obtained.

5.3. Development of a model of variation of the flow in the valve
The line pressure drop is determined by the expression

$$\Delta P_L = \Delta P_{M} + \Delta P_{S} = \frac{\sum \xi \rho \cdot v^2}{2} + \rho \cdot L \cdot \frac{v^2}{2D} = v^2 \cdot \alpha,$$

where $\Delta P_{M}$ is the pressure drop in local resistances, Pa; $\Delta P_{S}$ is the pressure drop in straight pipeline sections, Pa; $\xi$ is the local hydraulic drag coefficient; $\rho$ is the flow density, kg/m$^3$; $v$ is the flow velocity in the pipeline, m/s; $L$ is the length of straight pipeline sections, m; $\lambda$ is the hydraulic friction coefficient; $D$ is the pipeline diameter, m; $\alpha$ is a coefficient.

The valve pressure drop

$$\Delta P_v = P_s - P_f + \Delta P_{hl} - \Delta P_l = \beta - v^2 \cdot \alpha,$$

where $P_s$ is the initial pipeline pressure, Pa; $P_f$ is the final pipeline pressure, Pa; $\Delta P_{hl}$ is the hydrostatic pressure, Pa; $\Delta P_l$ is the line pressure drop, Pa; $\beta$ is the auxiliary coefficient.

The hydraulic index is determined by the relationship:

$$n = \frac{\Delta P_l}{\Delta P_v} = \frac{v^2 \cdot \alpha}{\beta - v^2 \cdot \alpha} = \frac{1}{\gamma/Q^2 - 1},$$

where $\gamma$ is the auxiliary coefficient; $Q$ is the volumetric flow rate of the medium, m$^3$/s.

$$\frac{Q^2}{Q_{max}^2} = \gamma / \gamma' + \frac{1}{1 + K - 1}.$$

where $Q_{max}$ is the maximum flow of the medium through the valve for the assumed throughput capacity of the valve $K_v$, m$^3$/s; $S$ is the valve opening rate, $(0<S<1)$; $d$ is the flow characteristic shape factor, taken to be 3.91.

The maximum flow in the system will occur with a fully open valve:

$$Q_{max} = 3.2 \sqrt{\frac{\Delta P}{\rho} + \left(\frac{1}{Kv} \right)^2} + \left(\frac{1}{Kv} \right)^2,$$

5.4. Automation equipment modeling
For the implementation of the developed control system, the latest automation equipment with the field interface RS485 Modbus [20] is chosen and its models are developed. The technical structure of the developed control system is shown in Fig. 2.

The continuous reactor is equipped with temperature measuring sensors for measuring the temperature of the nitration process and the temperature of the jacket cooling water. The ultrasonic level sensors and concentration meter provide continuous measurement of the level and concentration of nitropyridone. The data on the measured parameters...
are input to the industrial computer, which implements the algorithm of the developed reactor control system. The controls are fed to the object input through the actuators Ram. Tek.L.3500 and controllers.

5.5. Development of a precise control system of the vitamin B₆ production reactor

An object in the ACS is described by a system of nonlinear equations (1), supplemented by mathematical models of the equipment developed in section 5.4.

For the object control, a multivariable linear optimal digital controller with a model of step disturbances was chosen. The controller design is in accordance with the procedure described in [21, 22]. The model of the developed digital controller has the following form:

\[
\chi_{i+1} = A_z \chi_i + B_z (z_i - y_i),
\]

\[
u_i = C_z \chi_i,
\]

where \(z_i\) is the level setting in the reactor; \(z_3\) is the output product concentration setting; \(z_3\) is the temperature setting in the reactor.

Block diagrams of models for a simplified and accurate modeling of the developed ACS of the vitamin B₆ production reactor are shown in Fig. 3, a, b.

![Fig. 2. Technical structure of the control system](image)

![Fig. 2. Technical structure of the control system](image)

![Fig. 3. Block diagram of the control system modeling: a – simplified system; b – designed system; 1 – optimal multivariable controller; 2 – run-down actuator model; 3 – backlash actuator model; 4 – valve model; 5 – disturbance; 6 – uniform distributed random process simulating the control error; 7 – nonlinear model of the chemical reactor; 8 – uniform distributed random process simulating the sensor error; 9 – sensor model; 10 – system process logger](image)
The transients obtained by modeling of the designed control system are shown in Fig. 4.

Despite the imperfection of the automation equipment, the designed precise ACS of the vitamin B₆ synthesis process ensures not only the high quality of the vitamin, but also the synthesis process safety.

The results of the research are recommended for use in the pharmaceutical and chemical industries for the synthetic production of vitamin B₆. Also, the results can be useful for the research organizations that are engaged in the design of digital precise control systems.

A certain drawback of the research is that the developed approach to the synthesis of precise control systems was applied only to the design of a precise control system of the vitamin B₆ production reactor. Further improvement of the above approach involves the design of precise control systems for other industrial plants.

6. Discussion of the results of objectives accomplishment in the design of precise control systems of nonlinear objects

The approach to the design of precise control of industrial plants and math-ware for this approach in the form of a set of models are developed. Based on the approach, a precise automated control system of the vitamin B₆ synthesis reactor is developed. It can be seen that the characteristic feature of the proposed approach, which accounts for nonlinear properties of the ACS components, is getting more reliable results of modeling.

The analysis of the graphs in Fig. 4 shows that precise modeling of the automated control system yields the results that differ from the simplified system representation during the modeling. In addition to accurate simulation of the nonlinear model of the control object, accurate simulation of the real characteristics of the control equipment is also important in the design.

7. Conclusions

1. The model of a pharmaceutical chemical reactor for vitamin B₆ synthesis, considering the mutual influence of the parameters, thermodynamics, kinetics and order of the chemical reaction in accordance with the standards for chemical reaction modeling is developed.

2. The model of the influence of the controller characteristics on the flow of control fluid, which is characterized by the accounting of the nonlinear relationship between the flow rate and the controller opening rate is developed.

3. The model of the variation of the hydraulic friction coefficient with the flow of the medium is developed. The model is based on the approximation of the Colebrook-White nomogram. A high degree of coincidence of the model with the original is shown. The advantage of the developed model of accounting for the variation of the hydraulic friction coefficient is the possibility of using it directly in the control process.

4. The model of automation equipment, the distinctive feature of which is the accounting for operating characteristics of real equipment such as error, inertia, lag, backlash, run-down and the number of switches is developed.

5. The precise automated control system of the vitamin B₆ synthesis reactor is developed. The multivariable optimal controller is designed. Due to small deviations of transients under the action of disturbances, the proposed precise automated control system ensures the high quality of the product and process safety in the reactor. The developed set of models was used in the controller design and modeling.
References


