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MODELING AND OPTIMIZATION OF SILICA PRECIPITATION USING A LINEAR-QUADRATIC REGULATOR CONTROLLER

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Sulfuric acid precipitation of silica is a complex multistage process accompanied by intense exothermic reactions and rapid changes in the composition of the reaction mass. One of the key factors determining the quality and dispersion of the resulting silicon dioxide is temperature. Even slight deviations in the temperature regime lead to a change in the rate of polycondensation and, as a result, to a deterioration in the properties of the precipitate. To maintain process stability, a controller is required that can respond instantly to changes in state parameters and ensure optimal control of the reaction mixture heating. The paper develops a mathematical model of the sulfuric acid precipitation of silica in a continuous stirred tank reactor and implements a linear-quadratic regulator (LQR) that stabilizes the temperature near the operating point. Numerical modeling of the dynamics of concentrations and temperature under various acid supply modes was performed. It is shown that the use of an LQR controller effectively compensates for thermal disturbances, preventing overheating of the reaction mass and ensuring a stable reaction. The results confirm the feasibility of using LQR control to optimize and automate the processes of precipitated silica synthesis.

Keywords: sulfuric acid precipitation, silica, silicon dioxide, SiO_2 polycondensation, mathematical model, linear-quadratic controller.

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Introduction

Precipitated silica is a chemical frequently used as a reinforcing filler in polymer (elastomer) composites [1,2]. Its production is accomplished by acidifying an alkali silicate solution in a batch reactor. The reaction proceeds in the liquid phase with reversible properties, under isothermal, non-adiabatic conditions.

According to the literature [3–7], the key parameter determining the morphology, degree of aggregation, and specific surface area of precipitated SiO_2 is the temperature in the precipitation zone: increasing it typically leads to particle coarsening and a decrease in the sorption properties of the material. Calculations show that feeding a stoichiometric amount of acid into a 3-liter reactor results (under adiabatic conditions) in a temperature increase of ~18.1^{0}C. The exothermic nature of the neutralization reaction makes the process sensitive to the method of acid introduction and the heat removal mode.

Thus, maintaining the temperature within the optimal range (approximately 82^{0}C) is critical to ensuring the desired dispersion characteristics of the final product, such as average particle size and specific surface area. Exceeding the permissible temperature

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leads to particle coagulation and a decrease in silica quality, which limits its further application, particularly in sorption and catalytic systems. Conversely, decreasing the temperature reduces the rate of formation of SiO_2 nucleating particles and leads to a deterioration in the monodispersity of the product.

A partial solution to this problem is to spread out the acid feed over time. If the acid is fed very slowly, heat is released gradually over time, during which time some of the energy will be lost. In this case, the peak temperature is lower than in the adiabatic instantaneous case. However, this method does not completely eliminate uncontrolled temperature increases.

One way to stabilize the temperature is to use a PID controller, which allows the heater to be turned on until the temperature reaches a predetermined level. In this case, it is necessary to provide powerful cooling when the temperature is exceeded. Furthermore, a PID controller cannot account for the interactions between the system variables (monomer concentration, silica concentration, and temperature), and it is also difficult to optimize control between heating and acid feed rate.

An LQR controller has an advantage over a PID controller, allowing for optimal control in multiparameter processes with thermal and chemical dynamics [8]. This controller allows for rigid stabilization of the output parameter (in this case, temperature) while taking into account other state parameters.

The nonlinear nature of chemical processes and the complexity of analyzing experimental data obtained in studying sulfuric acid silica precipitation dictate the existence of multiple approaches to mathematical modeling. This, in turn, leads to high uncertainty and variability in model parameters when identifying them and using them for control problems. This paper examines a basic mathematical model approximating the chemical reactions occurring during the sulfuric acid precipitation of silica. It is used as a starting platform for researching and testing optimal control algorithms, as well as for evaluating their performance compared to traditional PID controllers widely used in industrial practice.

In recent years, methods based on optimal control and model-based approaches have been actively developed for solving process control problems in perfectly stirred tank reactors (CSTR). A significant role among these is played by the linear-quadratic controller (LQR), a fundamental tool in optimal control theory that has found wide application, including in chemical engineering [9]. LQR-based control involves minimizing a quadratic performance functional using feedback on the system's state vector, ensuring stable maintenance of process parameters near setpoints.

The aim of this work is to analyze the efficiency of LQR control for the process of sulfuric acid precipitation of silica, as well as to substantiate the feasibility of using optimal control methods in the design of automatic control systems in the production of precipitated silica.

Experimental

This paper examines the sulfuric acid precipitation of silica from a sodium silicate solution with a density of 1.08 g/cm^3, occurring at a temperature of 82^{0}C and a pressure of 1 atm [7] in a closed reactor with stirring. The reaction mixture volume is assumed to be constant, and mass transfer and evaporation are negligible. The starting sodium silicate (liquid glass) had a modulus of 3. The dry matter content was 37%. The calculated chemical formula is $Na_2O{\cdot}3SiO_2{\cdot}23H_2O$.

The mechanism of the process involves two following main reactions:

1. Acid decomposition of sodium silicate with the formation of monomer:

$$Na_2O{\cdot}3SiO_2{\cdot}23H_2O+H_2SO_4=Na_2SO_4+3H_4SiO_4+ +18H_2O. \quad (1)$$

2. Polycondensation of orthosilicic acid with the formation of SiO_2 sol:

$$H_4SiO_4=SiO_2+2H_2O. \quad (2)$$

The first reaction (1) is the acidic decomposition of sodium silicate upon contact with the silicate solution. The second reaction (2) is the polycondensation of orthosilicic acid, which is rate-controlling and determines the rate of silicon dioxide accumulation.

Both reactions are exothermic. Thermodynamic calculations of the enthalpies of reactions (1) and (2) at 82^{0}C give −162.91 kJ/mol and −15.07 kJ/mol, respectively.

For the system under consideration, let us introduce the following notations: concentration of sulfuric acid is C_H; concentration of orthosilicic acid monomer is C_m; and concentration of solid silicon dioxide is C_s.

The following balance equations can be written in terms of concentrations (mol·L^{-1}):

$$\frac{dC_H}{dt} = -r_1, \quad \frac{dC_m}{dt} = 3r_1 - r_2, \quad \frac{dC_s}{dt} = r_2, \quad (3)$$

where r_1 is the reaction (1) rate (mol·L^{-1}·s^{-1}); r_2 is the reaction (2) rate (mol·L^{-1}·s^{-1}).

The coefficient 3 in the equation for the monomer reflects the stoichiometry of reaction (1): one mole of sulfuric acid produces three moles of orthosilicic acid.

The following assumptions were made in the study:

– Reaction (1) occurs instantaneously, and its rate can be considered proportional to the rate of acid feed into the reactor:

$$r_1(t) = \frac{F_H(t)}{V}, \quad (4)$$

where $F_H(t)$ is the instantaneous consumption of sulfuric acid (mol·s^{-1}); V is the volume of the reaction mixture (L).

This approximation is valid because the acid concentration in the solution does not have time to increase significantly: it immediately reacts with the sodium silicate.

– Reaction (2) describes the polycondensation of the monomer H_4SiO_4 with the formation of solid silicon dioxide and is limiting. Its rate is described by a first-order equation for the monomer[7]:

$$r_2(t) = k(T) \cdot C_m(t), \quad (5)$$

where:

$$k(T) = A \cdot \exp(-\frac{E_a}{RT}). \quad (6)$$

Here A is the pre-exponential factor (s^{-1}); E_a is the activation energy (J·mol^{-1}); R is the universal gas constant (J·(mol·K)$^{-1}$); T is the reaction mass temperature (K).

We consider the formation of silicon dioxide (reaction (2)) to be irreversible:

$$\frac{dC_s}{dt} = r_2; \quad r_{2reverse}=0.$$

– The sodium silicate concentration is not considered explicitly, since it is completely consumed in monomer formation during reaction (1);

– When modeling acid supply, the function $F_H(t)$ is set as a constant for a specified dosing time, after which it returns to zero.

Thus, taking into account expressions (3), (4), and (5), the system of differential equations for reactor concentrations is as follows:

$$\left\{\begin{array}{l} \frac{dC_H}{dt} = -\frac{F_H(t)}{V}, \\ \frac{dC_m}{dt} = 3\frac{F_H(t)}{V} - k(T)C_m \\ \frac{dC_S}{dt} = k(T)C_m \end{array}\right\}$$

This nonlinear system describes the dynamics of chemical transformations during sulfuric acid precipitation of silica and serves as the basis for further construction of the heat balance and calculation of the control action. The thermal behavior of the system during sulfuric acid precipitation of silica is determined by the total balance between the heat supplied by the heater, the heat released by chemical reactions (1) and (2), and heat losses to the environment.

The heat balance equation can be written as follows:

$$C_{th}\frac{dT}{dt} = Q_H(t) + Q_{rxn}(t) - Q_{loss}(t),$$

where C_{th} is the effective heat capacity of the reaction mass (J·K^{-1}); T is the current reactor temperature (K); $Q_H(t)$ is the heating capacity of the heater (J·s^{-1}); $Q_{rxn}(t)$ is the thermal effect of reactions (1) and (2) (J·s^{-1}); $Q_{loss}(t)$ is the heat loss (J·s^{-1}).

The heat supplied by an electric heater with power P_{max} and control signal u(t) ($0 \le u \le 1$) is described as follows:

$$Q_H(t) = u(t)P_{max}.$$

The thermal effect of chemical reactions consists of two following contributions:

1. Reaction (1) – instantaneous interaction of acid with sodium silicate occurs synchronously with the supply of acid; the heat released is expressed as:

$$Q_{r_1}(t) = -\Delta H_1 F_H(t) \quad (7)$$

where ΔH_1 is the heat effect of reaction (1) (J·mol^{-1}); $F_H(t)$ is the sulfuric acid consumption (mol·s^{-1}).

2. Reaction (2) – polycondensation of orthosilicic acid. The rate of heat release is proportional to the reaction rate $r_2(t)=k(T)C_m(t)$:

$$Q_{r_2}(t) = -\Delta H_2 V r_2(t) = -\Delta H_2 V k(T) C_m(t), \quad (8)$$

where ΔH_2 is the heat effect of polycondensation (J·mol^{-1}).

Total thermal effect of reactions:

$$Q_{rxn}(t) = Q_{r_1}(t) + Q_{r_2}(t). \quad (9)$$

Heat exchange with the environment is approximately described by a linear law:

$$Q_{loss}(t) = H(T - T_a), \quad (10)$$

where H is the effective heat transfer coefficient ($W \cdot K^{-1}$); T_a is the ambient temperature (K).

As a result, after substituting expressions (6)–(10) we obtain the heat balance equation:

$$C_{th}\frac{dT}{dt} = u(t)P_{\max} - H(T - T_a) - \Delta H_1 F_H(t) - \Delta H_2 V k(T) C_m(t).$$

This equation describes the dynamics of changes in the temperature of the reaction mass under the influence of both controlled heating and internal exothermic processes.

The complete dynamics of the chemical-thermal model can be described by the following system:

$$\begin{cases} \frac{dC_H}{dt} = -\frac{F_H(t)}{V} \\ \frac{dC_m}{dt} = 3\frac{F_H(t)}{V} - k(T)C_m \\ \frac{dC_s}{dt} = k(T)C_m \\ C_{th}\frac{dT}{dt} = u(t)P_{\max} - H(T - T_a) - \Delta H_1 F_H(t) - \Delta H_2 V k(T) C_m \end{cases}. \quad (11)$$

This nonlinear system of equations (11) completely describes the interrelated dynamics of reactant concentrations, solid silica accumulation, and temperature changes during the sulfuric acid precipitation process. It serves as the basis for developing a reactor temperature control model and analyzing the effect of acid dosing on the system's thermal stability.

However, the LQR controller is linear and is applied to linear or weakly nonlinear models. Analysis of the silica precipitation process revealed that this system exhibits a number of nonlinearities:

– the exponential dependence of the reaction rate coefficient on temperature (6);

– the reaction rate, equation (2), is calculated by multiplying the state function T by the state C_m, i.e., $r_2 = C_m k(T)$, which results in nonlinearity;

– when calculating the enthalpy, equation (2), it is necessary to take into account the product $C_m k(T)$, which is also nonlinear.

Other potential nonlinearities, such as changes in heat capacity with temperature, changes in density and volume, nonlinear heat loss models, etc., are neglected. The system belongs to the class of multi-nonlinear dynamic systems, where nonlinearity manifests itself in thermal and kinetic dependencies. Thus, to implement an LQR controller, several tasks must be solved:

– formulate the states and inputs:

$$x = [C_m, C_s, T, C_H]^T, \; u = [u_1, u_2]^T,$$

where u_1 is the heating; u_2 is the acid supply;

– perform linearization at the operating point: x_0, y_0;

– assess the controllability of the model: ensure that matrices A and B are controllable, where A is the state matrix, B is the control matrix;

– select the optimal Q and R matrices, where Q is the weight matrix of states, R is the weight matrix of control.

The initial parameters are given in Table.

To create an LQR control model, let us represent the nonlinear system (10) in matrix form:

$$\dot{x} = A(x)x + B(x)u, \; y = Cx + Du.$$

There are three state variables: monomer concentration C_m, solid accumulation C_S and temperature T.

Two control inputs, heating control signal $u_1(t)$ ($0 \le u_1 \le u_1 \le 1$) and acid supply $u_2(t) = F_H(t)$.

Thus, in matrix form:

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} C_m \\ C_s \\ T \end{bmatrix}, \quad u_v = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} u_1(t) \\ F_{H_2SO_4}(t) \end{bmatrix},$$

$$\dot{x} = f(x,u),$$

and the nonlinear equations on the right-hand sides have the form:

$$\dot{x}_1 = -k(x_3)x_1 + \frac{3}{v}u_2(t),$$

$$\dot{x}_2 = k(x_3)x_1,$$

$$\dot{x}_3 = -\frac{\Delta H_2 V}{C_{th}}k(x_3)x_1 - \frac{H}{C_{th}}(x_3 - T_a) + \frac{P_{\max}}{C_{th}}u_1(t) - \frac{\Delta H_1}{C_{th}}u_2(t).$$

State matrix A:

$$A = \begin{bmatrix} -k(x_3) & 0 & 0 \\ k(x_3) & 0 & 0 \\ -\frac{\Delta H_2 V}{C_{th}}k(x_3) & 0 & -\frac{H}{C_{th}} \end{bmatrix}$$

Input matrix B:

$$B = \begin{bmatrix} 0 & \frac{3}{V} \\ 0 & 0 \\ \frac{P_{\max}}{C_{th}} & -\frac{\Delta H_1}{C_{th}} \end{bmatrix}$$

LQR synthesis requires a linear model around the operating point (x_0, u_0). Select the mode at which the temperature T_0=355.15 K, and the serving u_2 taken as equal to the nominal value $F_H(t)$. Working point of states C_{m0}=0, C_{s0}=0.

Linearization is performed as standard using first-order Taylor series around (x_0, $u_{0)}$). Let us denote k_0=k(T_0), then we have:

$$\left.\frac{dk}{dt}\right| T_0 = k_0 \frac{E_a}{RT_0^2} \equiv k_T .$$

Functions of the right-hand sides are as follows:

$$f_1(C_m, C_s, T, u_1, u_2) = 3u_2 - k(T)C_m,$$

$$f_2(C_m, C_s, T, u_1, u_2) = k(T)C_m,$$

$$f_3(C_m, C_s, T, u_1, u_2) = \\ = \frac{1}{C_{th}}(u_1 P_{max} - H_{loss}(T - T_a) - \Delta H_1 V u_2 - \Delta H_2 V k(T) C_m) .$$

Jacobians by state x and by the control vector u have the following appearance:

Matrix $A = \left.\frac{\partial f}{\partial x}\right|_{x_0 u_0}$

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial C_m} & \frac{\partial f_1}{\partial C_s} & \frac{\partial f_1}{\partial T} \\ \frac{\partial f_2}{\partial C_m} & \frac{\partial f_2}{\partial C_s} & \frac{\partial f_2}{\partial T} \\ \frac{\partial f_3}{\partial C_m} & \frac{\partial f_3}{\partial C_s} & \frac{\partial f_3}{\partial T} \end{bmatrix}_{(x_0 u_0} =$$

$$= \begin{bmatrix} -k_0 & 0 & -C_{m0}k_T \\ k_0 & 0 & C_{m0}k_T \\ -\frac{\Delta H_2 V}{C_{th}}k_0 & 0 & -\frac{H_{loss}}{C_{th}} - \frac{\Delta H_2 V}{C_{th}} C_{m0}k_T \end{bmatrix}$$

where $\partial f_1 / \partial C_m = -k_0$, $\partial f_1 / \partial T = -C_{m0} dk/dT = -C_{m0}k_T$.

Initial parameters

Parameter	Designation	Value	Dimensionality
Reactor volume	V	0.003	m^3
Solution density	ρ	1080	kg/m^3
Mass of solution	M	3.24	kg
Heat capacity	C_P	4180	J/(kg·K)
Total heat capacity of the solution	C_S	13543	J/K
Molecular weight (sodium silicate)	M_{CH}	0.6566	kg/mol
Quantity (sodium silicate)	m_{CH}	0.2578	kg
Amount of acid (in 3 liters)	m_H	0.1272	kg
Acid feed rate	F_H	$2.653 \cdot 10^{-4}$	mol/s
Operating point temperature	T_0	82	^0C
Pre-exponential reactions (2)	A	2583.3	1/s
Reaction activation energy (2)	E_a	44900	g/mol
Gas constant	R_a	8.314	J/(mol·K)
Enthalpy of reaction (1)	ΔH_1	–162910	g/mol
Enthalpy of reaction (2)	ΔH_2	–15070	g/mol
Maximum heater power	P_{max}	1000	W
Ambient temperature	T_a	25	^0C
Acid delivery time	t_p	4440	s
Heat loss	H	15	$W \cdot K^{-1}$

Matrix $B = \frac{\partial f}{\partial u}\Big|_{x_0 u_0}$

$$B = \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \\ \frac{\partial f_3}{\partial u_1} & \frac{\partial f_3}{\partial u_2} \end{bmatrix}_{(x_0 u_0)} = \begin{bmatrix} 0 & 3 \\ 0 & 0 \\ \frac{P_{\max}}{C_{th}} & -\frac{\Delta H_1 V}{C_{th}} \end{bmatrix}.$$

To analyze the applicability of LQR, it is necessary to verify the controllability of the linear model. Controllability is verified by the rank of the Kalman matrix:

$$U = \left[B \; AB \; A^2 B\right]. \quad (12)$$

If rank n (here n=3), the system is controllable. In the case of two inputs, B has two columns—this increases the chances of complete controllability; if an LQR is designed for only one input (for example, u_1), the check is performed against the corresponding column B1. The performance indicator of the LQR controller is determined as follows:

$$J = \int_0^\infty (x^T Q x + u^T R u) dt,$$

where Q≥0 and R>0 set preferences (penalties) for deviations in states and energy consumption, respectively. To achieve optimal control, the value of J must be minimal.

To design an LQR controller, we set positive definite matrices Q and R:

$$Q = \begin{bmatrix} 100 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 1000 \end{bmatrix}, \quad R = 10.0$$

It should be noted that there is no single method for adjusting these parameters. Usually, trial and error is used to select the correct parameters. We have chosen a large value for the temperature component (1000), which makes the controller sensitive to temperature deviations and acts intensively on u_1, to keep T close to T_0.

Results and discussion

To determine the numerical values of matrices A and B, as well as the optimal feedback matrix *K* for the LQR controller, it is necessary to calculate the elements of the matrices:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix},$$

where

$$a_{11} = -k_0, a_{12} = 0, a_{13} = -C_{m0} k_T, a_{21} = k_0, a_{22} = 0, a_{23} = C_{m0} k_T,$$
$$a_{31} = -\frac{\Delta H_2 V}{C_{th}} k_0, a_{32} = 0, a_{33} = -\frac{H_{loss}}{C_{th}} - \frac{\Delta H_2 V}{C_{th}} C_{m0} k_T.$$

$$B = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \end{bmatrix},$$

where

$$b_{11} = 0, b_{12} = 3, b_{21} = 0, b_{22} = 0, b_{31} = \frac{P_{\max}}{C_{th}}, b_{32} = -\frac{\Delta H_1 V}{C_{th}}.$$

After calculating the elements of matrices A and B, we obtain:

$$A = \begin{bmatrix} -6.429 \cdot 10^{-4} & 0.0 & -1.136 \cdot 10^{-5} \\ 6.429 \cdot 10^{-4} & 0.0 & 1.136 \cdot 10^{-5} \\ 2.146 \cdot 10^{-3} & 0.0 & -1.069 \cdot 10^{-3} \end{bmatrix},$$

$$B = \begin{bmatrix} 0 & 3.0 \\ 0 & 0 \\ 0.0738 & 36.087 \end{bmatrix}.$$

To find the optimal control action $K=R^{-1}B^TPA$ computer program was written in Python, in which the algebraic Riccati equation was solved with weights Q=diag(100, 10, 1000), R_scalar=10:

$A^TP+PA-PBR^{-1}B^TP+Q=0$,

and the input controller matrix is calculated u_1:

$K=[2.11 \cdot 10^{-2}, 1.77 \cdot 10^{-3}, 9.98 \cdot 10^{0}]$,

as well as proper numbers for a system with feedback on u_1 ($A_{cl}=A-B_1K_1$):

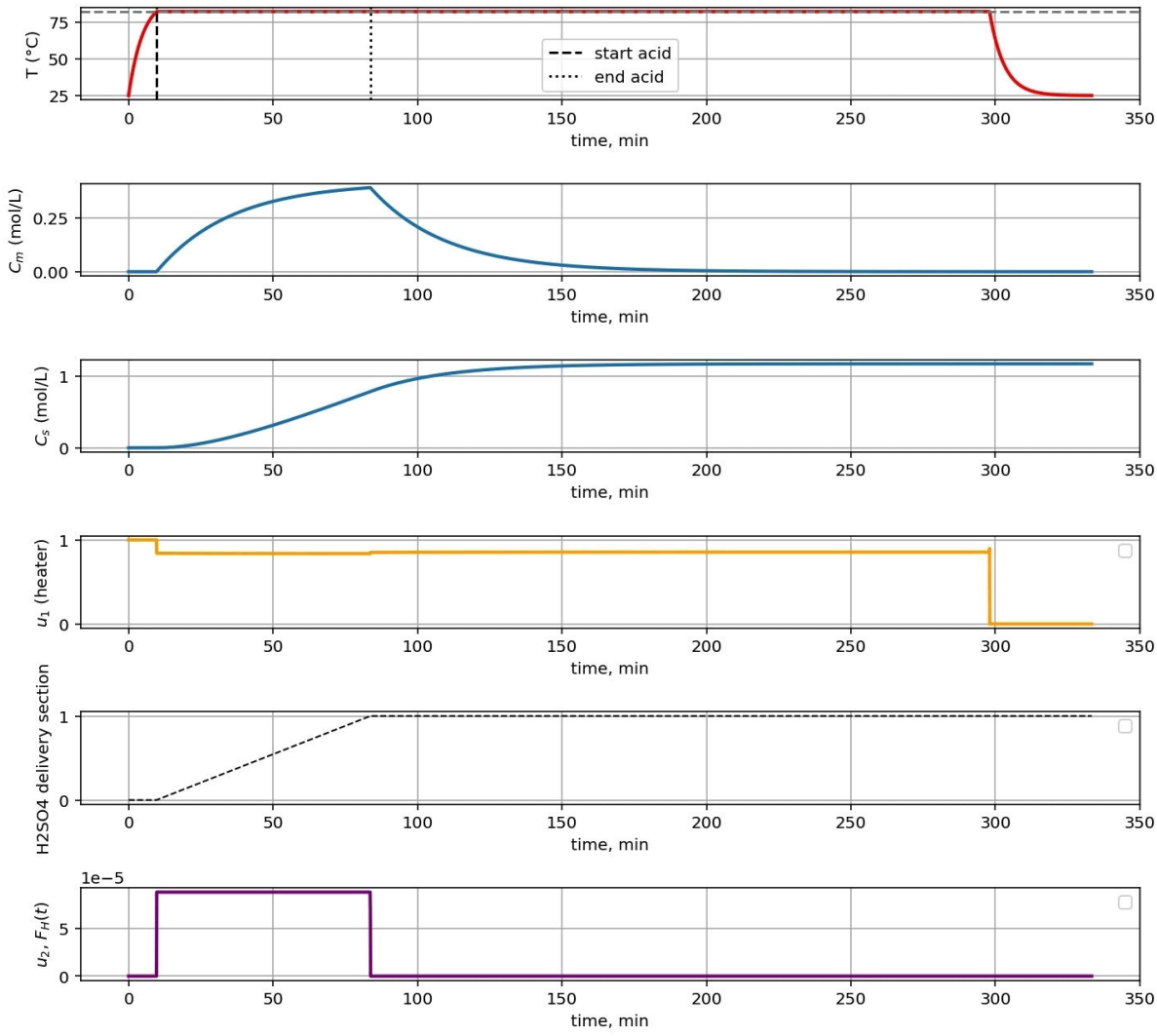
$\lambda(A_{c1}) \approx -0.74; -6.43 \cdot 10^{-4}; 1.33 \cdot 10^{-17}$.

The controllability matrix rank calculated using formula (11) is equal to 2, i.e. a single heater cannot fully control all three states. u_1 acts directly only on temperature through the heat balance. This can be seen from the eigenvalues of the closed system. The intrinsic number $\lambda \approx -0.74$ s^{-1} corresponds to the rapid response of the controlled heater. At the same time, small values of C_m and especially C_s indicate a weak relationship between u_1 and concentrations, possibly only through the temperature dependence of the rate k(T). To control the concentrations, a second channel is required, direct acid supply u_2 as a controlled parameter, i.e. for complete control of the process, an integral controller with two inputs, u_1 and u_2 together, is required, but in this case it is not necessary because the main parameter, temperature, is strictly stabilized. This can be seen from the graphs shown in Figure.

The computer program provides for the addition of acid after the reaction mass reaches the specified temperature. According to calculations, this moment occurs at the 10-minute mark. The temperature of the reaction mass rises at the beginning of the process due to heating and stabilizes at around 82^0C. The smooth attainment of a steady state value indicates that the regulator is working correctly. Subsequently, the temperature does not change despite the thermal effects of reactions (1) and (2).

The concentration of monomer C_m increases during the acid supply period, reaches a maximum at the end of the supply, and then decreases due to polycondensation. After 150 minutes, the process stabilizes.

The sediment concentration C_S increases monotonically and reaches a horizontal plateau after



Results of modeling the sulfuric acid precipitation of silica: changes in the temperature of the reaction mass, concentrations of monomer and precipitate, as well as signals controlling heating and acid supply

150−200 minutes, which corresponds to the end of the reaction.

As can be seen from the graph, at the beginning of the process, the supplied heating power is maximum u_1=1. However, after the influence of exothermic reactions (1) and (2), the heater power decreases due to heat release. After the temperature stabilizes, the regulator maintains the minimum value u, compensating for heat loss.

The following figure shows the dynamics of sulfuric acid consumption. The curve increases linearly to 1 at the moment of completion of supply (≈100 min), which confirms uniform dosing. At the same time, acid consumption, u_2, has a step-like character: it is switched on at the beginning and switched off after 100 min, which corresponds to the planned mode.

Conclusions

1. Developed nonlinear model of sulfuric acid precipitation of silica adequately describes the dynamics of concentrations and temperature of the reaction mass.

2. The Q and R matrices are configured so that temperature deviations are most noticeable in the optimization function (12). This means that the calculated optimal control (13) almost completely compensates for all thermodynamic disturbances, and the temperature remains close to the calculated steady state point.

3. The neutralization reaction has a dominant influence on the thermal regime.

4. The LQR controller demonstrates good response and provides stable temperature stabilization near the operating point of 82^{0}C.

5. Full control of the process requires an advanced dual-channel controller for u_1 and u_2.

6. The model can be used to optimize acid dosing and design automatic control systems in the production of precipitated silica.

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МОДЕЛЮВАННЯ І ОПТИМІЗАЦІЯ ОСАДЖЕННЯ КРЕМНЕЗЕМУ З ВИКОРИСТАННЯМ ЛІНІЙНО-КВАДРАТИЧНИЙ РЕГУЛЯТОРА

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Сірчанокислотне осадження кремнезему є складним багатостадійним процесом, що супроводжується інтенсивними екзотермічними реакціями та швидкою зміною складу реакційної маси. Температура є одним з ключових факторів, що визначають якість і дисперсність кремній діоксиду, що осаджується. Навіть незначні відхилення температурного режиму призводять до зміни швидкості поліконденсації і, як наслідок, погіршення властивостей осаду. Для підтримки стабільності процесу потрібен регулятор, здатний миттєво реагувати на зміну параметрів стану та забезпечувати оптимальне керування нагріванням реакційної суміші. У роботі розроблено математичну модель процесу сірчанокислотного осадження кремнезему в реакторі ідеального змішування та реалізовано лінійно-квадратичний регулятор, що забезпечує стабілізацію температури поблизу робочої точки. Проведено чисельне моделювання динаміки концентрацій та температури за різних режимів подачі кислоти. Показано, що застосування лінійно-квадратичного регулятора дозволяє ефективно компенсувати теплові збурення, запобігаючи перегріву реакційної маси та забезпечуючи стійке проходження реакції. Отримані результати підтверджують доцільність використання лінійно-квадратичного регулювання для оптимізації та автоматизації процесів синтезу осадженого кремнезему.

Ключові слова: сірчанокислотне осадження, кремнезем, кремній діоксид, поліконденсація SiO_2, математична модель, лінійно-квадратичний регулятор.

MODELING AND OPTIMIZATION OF SILICA PRECIPITATION USING A LINEAR-QUADRATIC REGULATOR CONTROLLER

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Sulfuric acid precipitation of silica is a complex multistage process accompanied by intense exothermic reactions and rapid changes in the composition of the reaction mass. One of the key factors determining the quality and dispersion of the resulting silicon dioxide is temperature. Even slight deviations in the temperature regime lead to a change in the rate of polycondensation and, as a result, to a deterioration in the properties of the precipitate. To maintain process stability, a controller is required that can respond instantly to changes in state parameters and ensure optimal control of the reaction mixture heating. The paper develops a mathematical model of the sulfuric acid precipitation of silica in a continuous stirred tank reactor and implements a linear-quadratic regulator (LQR) that stabilizes the temperature near the operating point. Numerical modeling of the dynamics of concentrations and temperature under various acid supply modes was performed. It is shown that the use of an LQR controller effectively compensates for thermal disturbances, preventing overheating of the reaction mass and ensuring a stable reaction. The results confirm the feasibility of using LQR control to optimize and automate the processes of precipitated silica synthesis.

Keywords: sulfuric acid precipitation; silica; silicon dioxide; SiO_2 polycondensation; mathematical model; linear-quadratic controller.

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