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OPTIMAL CONTROL OF BENZENE ALKYD PROCESS BY PROPYLENE IN LIQUID PHASE

Summary: The mathematical model of the process of benzene alkylation was developed in the liquid phase based on the use of tolerances. Suggested optimality criterion. Found the optimum control of benzene alkyd process in liquid phase. The optimum linear regulator is synthesized.

Keywords: process of benzene alkylability, mathematical model, optimality criterion, optimum control with feedback, matrix differential equation Rikatti

OPTIMALNE STEROWANIE PROCESEM ALKILOWANIA BENZENU Z PROPYLENEM W STANIE CIEKŁYM

Streszczenie: Opracowano model matematyczny dla procesu alkilowania benzenu w stanie ciekłym, z zastosowaniem tolerancji. Zaproponowano kryteria optymalizacji. Znalaziono optymalny proces sterowania alkilowania benzenu w stanie ciekłym. Zrealizowano syntezę optymalną regulatora liniowego.

Słowa kluczowe: proces alkilowania benzenu, model matematyczny, kryterium optymalizacji, sterowanie optymalne ze sprzężeniem zwrotnym, macierz równań różniczkowych Rikatti

1. Introduction

Benzoin benzene is carried out in order to obtain Isopropyl benzol. The process of benzene alkylation is very intense, the temperature is determined by the supply

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of propane-propylene fraction in the alkylator, the heat is allocated by evaporation of benzene excess, as well as cooling water.

The main reaction apparatus is alkylator. It is a column inside the lining graphite tiles. Alkylator top filled with a mixture of benzene and solution catalyst. The lower part of the machine continuously serves drained benzene, catalyst and gaseous propane-propylene fraction containing 30... 40% propylene. The calculation scheme of the alkylator is shown in Figure 1:

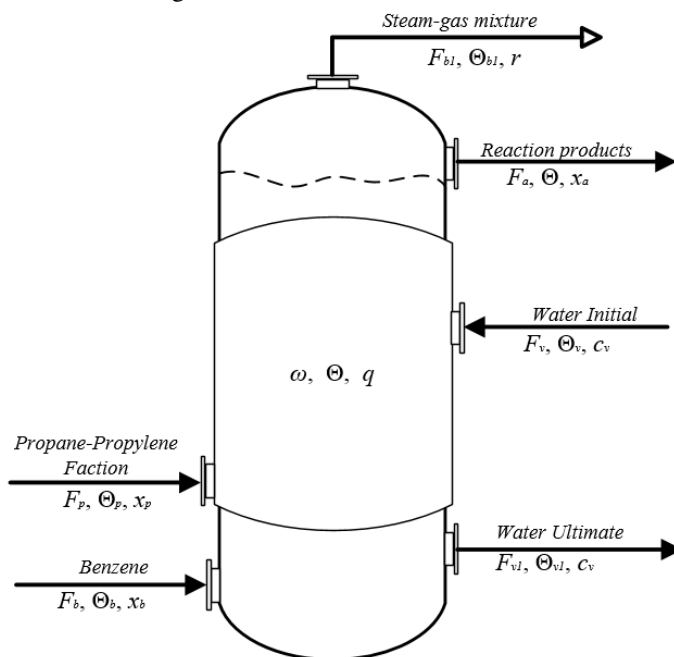


Figure 1. Structural-parametric scheme of Alkylator

$F_b, F_{bl}, F_p, F_a, F_v, F_{vl}$ – consumption of benzene at the entrance to the machine and fired; propylene reaction products; water on inlet and outlet cooling; kg/s; $\Theta_b, \Theta_p, \Theta_{bl}, \Theta, \Theta_v, \Theta_{vl}$ – temperature of benzene and propylene; gas mixture; reactional mass in reactor; water inlet and outlet; K; x_b, x_p, x_a – the concentration of benzene and propylene at the inlet and alkylate at the output; %; q – specific heat of reaction; J/kg; c_v – specific heat capacity of water; J/(kg·K); ω – speed of reaction; m/s; r – the specific heat of the steamer benzoyl; J/kg.

Disturbance: Water temperature.

Control effect: Water consumption, the consumption of propylene (in this paper is considered only the control of the cost of propane-propylene fraction, as it is the most optimum).

Adjustable value: alkylite temperature, Alkylat concentration.

The main purpose of optimum control is to maintain a predetermined temperature and the concentration of alkylate at the output from the machine at minimizing the cost of propane-propylene fraction.

Proceeding from this, we introduce a criterion of optimality:

$$I = \frac{1}{2} \int_0^{t_f} [q_{11}(x_a - x_a^{3d})^2 + q_{22}(\Theta - \Theta^{3d})^2 + r \cdot F_p^2] dt \rightarrow \min$$

where q_{11} , q_{22} , r – weighing coefficients.

Mathematical model for Alkylator was created for calculation of optimum control system. In which the data of assumptions were taken into:

1. Volume of liquid in alkylator sustainable – $v = const$.
2. Lack of heat loss in the environment.
3. The temperature in the apparatus and at the exit from it will be the same $\Theta_a = \Theta_{p1} = \Theta_{b1} = \Theta$.

2. Material balance for the acoustic capacity of the reactional mass in alkylator at the values of concentration

$$-F_a \cdot x_a + v \cdot \rho \cdot \omega = v \cdot \rho \frac{dx_a}{dt} \quad (1)$$

Since the reaction has the first order, its speed will be determined by the concentration of propane-propylene fraction x_{p1} in the reactor, i.e. propane that did not react. Given the law of Arrhenius and the law of the masses, the reaction rate equals:

$$\omega = \frac{M_a}{M_p} k \cdot \exp\left(-\frac{E}{R(273+\Theta)}\right) \cdot x_{p1} \quad (2)$$

M_a and M_p – the molar masses of alkylite and propylene in accordance with.

Where $x_{p1} = \frac{1}{F_a} (F_p x_p - \frac{M_p}{M_a} x_a) = \frac{F_p}{F_a} x_p - \frac{M_p}{M_a} x_a$.

By technology:

$$F_b = m \cdot F_p$$

m – cost ratio of propylene to benzene ($m=2$).

For simplification of calculations and lyunization the equation will use the mathematical formula in compliance with our equation and the data which must be expressed:

$$\frac{\partial f}{\partial x} \cdot \frac{\partial x}{\partial t} = \frac{\partial f(F_p, \Theta, x_a)}{\partial F_a} \cdot \frac{\partial F_a}{\partial x_a} \cdot \Delta x_a$$

Find:

$$\left. \frac{\partial f(F_p, \Theta, x_a)}{\partial F_a} \right|_0 = -x_a \Big|_0$$

$$\left. \frac{\partial F_a}{dx_a} \right|_0 = \frac{\frac{M_b}{M_a} F_p (m+1-m \cdot x_b)}{\left(1 - \frac{M_b}{M_a} x_a\right)^2} \Bigg|_0$$

M_b – molar mass of benzene.

Substituting all expressions, get:

$$\Delta x_a \left[-x_a \cdot \frac{M_b \cdot M_a \cdot F_p (m+1-m \cdot x_b)}{(M_a - M_b \cdot x_a)^2} + A_1 \left(\frac{-M_b \cdot x_p}{M_a (m+1-m \cdot x_b)} + \frac{M_p}{M_a} \right) \right] \Bigg|_0 = -A_2 \cdot \Delta x_a$$

Enter some designations:

$$A_1 = v \cdot \rho \cdot \frac{M_a}{M_p} k \cdot \exp\left(-\frac{E}{R(273+\Theta)}\right), \quad (3)$$

$$A_2 = -x_a \cdot \frac{M_b \cdot M_a \cdot F_p (m+1-m \cdot x_b)}{(M_a - M_b \cdot x_a)^2} + A_1 \left(\frac{-M_b \cdot x_p}{M_a (m+1-m \cdot x_b)} + \frac{M_p}{M_a} \right), \quad (4)$$

$$A_3 = \frac{M_b \cdot M_a \cdot F_p (m+1-m \cdot x_b)}{(M_a - M_b \cdot x_a)^2}, \quad (5)$$

$$A_4 = \frac{-M_b \cdot x_p}{M_a (m+1-m \cdot x_b)} + \frac{M_p}{M_a}. \quad (6)$$

Similarly to Θ :

$$\Delta \Theta \left[\frac{M_a}{M_p} k \cdot v \left(\frac{F_p}{F_a} x_p + \frac{M_p}{M_a} x_a \right) \cdot \exp\left(-\frac{E}{R(273+\Theta)}\right) \cdot \left(\frac{E}{R(273+\Theta)^2} \right) \right] \Bigg|_0 = A_5 \cdot \Delta \Theta$$

We introduce the symbol:

$$A_5 = \frac{M_a}{M_p} k \cdot v \left(\frac{F_p}{F_a} x_p + \frac{M_p}{M_a} x_a \right) \cdot \exp\left(-\frac{E}{R(273+\Theta)}\right) \cdot \left(\frac{E}{R(273+\Theta)^2} \right) \quad (7)$$

Substituting Expressions (3)-(7) in (1) and write the equations in increments and transfer the original parameters into the right part of the equation, and the incoming- to the left:

$$-A_2 \cdot \Delta x_a + A_5 \cdot \Delta \Theta = v \cdot \rho \frac{d\Delta x_a}{dt}$$

From here we write the equations in the state space for the material balance for the acoustic capacity of the reactional mass in the alkylator at the values of concentration:

$$\frac{\partial x_a}{\partial t} = a_{11} \cdot x_a + a_{12} \cdot \Theta,$$

$$\text{where } a_{11} = -\frac{A_4}{v \cdot \rho}; \quad a_{12} = \frac{A_5}{v \cdot \rho}.$$

3. Thermal balance of reactional mass

$$F_b \cdot c_b \cdot \Theta_b + F_p \cdot c_p \cdot \Theta_p - F_a \cdot c_a \cdot \Theta - KS \left(\Theta - \frac{\Theta_v + \Theta_{v1}}{2} \right) -$$

$$-F_{b1} \cdot r_b + v \cdot \omega \cdot q = v \cdot \rho \cdot c_a \frac{d\Theta}{dt}$$

In expression (2) we will make the notation and record the rate formula:

$$\frac{F_p}{F_a} = \frac{M_a - M_b \cdot x_a}{M_a(m+1-m \cdot x_b)} = f3(x_a),$$

$$\omega = \frac{A_1}{v \cdot \rho} \left(f3(x_a)x_p + \frac{M_p}{M_a} x_a \right). \quad (8)$$

Substituting (2) in the general expression of the thermal balance, we will have:

$$F_p(m \cdot c_b \cdot \Theta_b + c_p \cdot \Theta_p) - F_a \cdot c_a \cdot \Theta - KS \left(\Theta - \frac{\Theta_v + \Theta_{v1}}{2} \right) -$$

$$- \left(-\frac{M_b}{M_a} x_a \cdot F_a + m \cdot F_p \cdot x_b \right) \cdot r_b + v \cdot \frac{A_1}{v \cdot \rho} \left(f3(x_a)x_p + \frac{M_p}{M_a} x_a \right) \cdot q = v \cdot \rho \cdot c_a \frac{d\Theta}{dt}$$

Linearization of the thermal balance equation in the growth:

$$\Delta F_p \left[m \cdot c_b \cdot \Theta_b + c_p \cdot \Theta_p - c_a \cdot \Theta \frac{m+1-m \cdot x_b}{1-\frac{M_b}{M_a} x_a} - m \cdot x_b \cdot r_b \right] -$$

$$-\Delta \Theta \left[F_a \cdot c_a + KS + v \cdot q \cdot x_{p1} \frac{M_a}{M_p} k \cdot \exp \left(-\frac{E}{R(273+\Theta)} \right) \cdot \left(\frac{E}{R(273+\Theta)^2} \right) \right] +$$

$$+\Delta x_a \left[v \cdot q \cdot \frac{A_1}{v \cdot \rho} (A_5) - c_a \cdot \Theta \cdot A_6 + r_b \cdot \frac{M_b}{M_a} (F_a + x_a \cdot A_6) \right] + \Delta \Theta_{v1} \cdot \frac{KS}{2} + \Delta \Theta_v \cdot \frac{KS}{2}$$

$$=$$

$$= v \cdot \rho \cdot c_a \frac{d\Delta\Theta}{dt} \quad (9)$$

We introduce the symbol:

$$B1 = m \cdot c_b \cdot \Theta_b + c_p \cdot \Theta_p - c_a \cdot \Theta \frac{m+1-m \cdot x_b}{1-\frac{M_b}{M_a} x_a} - m \cdot x_b \cdot r_b, \quad (10)$$

$$B2 = F_a \cdot c_a + KS + v \cdot q \cdot x_{p1} \frac{M_a}{M_p} k \cdot \exp\left(-\frac{E}{R(273+\Theta)}\right) \cdot \left(\frac{E}{R(273+\Theta)^2}\right), \quad (11)$$

$$B3 = v \cdot q \frac{A_1}{v \cdot \rho} (A_5) - c_a \cdot \Theta \cdot A_6 + r_b \cdot \frac{M_b}{M_a} (F_a + x_a \cdot A_6), \quad (12)$$

$$B4 = \frac{KS}{2}. \quad (13)$$

Substituting expressions (10)-(13) in (9) get:

$$B1 \cdot \Delta F_p - B2 \cdot \Delta\Theta + B3 \cdot \Delta x_a + B4 (\Delta\Theta_{v1} + \Delta\Theta_v) = v \cdot \rho \cdot c_a \frac{d\Delta\Theta}{dt}.$$

So, we write the equations in the space of the thermal balance condition for the ozone mass:

$$\frac{\partial\Theta}{dt} = b_2 \cdot F_p + a_{22} \cdot \Theta + a_{21} \cdot x_a + a_{23} (\Theta_{v1} + \Theta_v)$$

$$\text{where } a_{21} = \frac{B_3}{v \cdot \rho \cdot c_a}; \quad a_{22} = \frac{-B_2}{v \cdot \rho \cdot c_a}; \quad a_{23} = \frac{B_4}{v \cdot \rho \cdot c_a}; \quad b_2 = \frac{B_1}{v \cdot \rho \cdot c_a}.$$

4. Thermal balance on the water temperature supplied on cooling

$$F_v \cdot c_v \cdot \Theta_v - F_v \cdot c_v \cdot \Theta_{v1} + KS \left(\Theta - \frac{\Theta_{v1} + \Theta_v}{2} \right) = v_v \cdot \rho_v \cdot c_v \frac{d}{dt} \left(\frac{\Theta_v - \Theta_{v1}}{2} \right)$$

Perform liunization equation:

$$\begin{aligned} \Delta F_v (c_v \cdot \Theta_v - c_v \cdot \Theta_{v1}) + \Delta\Theta_v \left(F_v \cdot c_v - \frac{KS}{2} \right) - \Delta\Theta_{v1} \left(F_v \cdot c_v + \frac{KS}{2} \right) + \Delta\Theta \cdot KS = \\ = \frac{v_v \cdot \rho_v \cdot c_v}{2} \left(\frac{d\Delta\Theta_v}{dt} + \frac{d\Delta\Theta_{v1}}{dt} \right). \end{aligned}$$

We introduce the symbol:

$$D1 = c_v \cdot \Theta_v - c_v \cdot \Theta_{v1}; D2 = F_v \cdot c_v - \frac{KS}{2}; D3 = F_v \cdot c_v + \frac{KS}{2}; D4 = KS.$$

So, we write the equations in the thermal balance condition space on the water temperature:

$$\frac{\partial \Theta_v}{dt} = a_{32} \cdot \Theta + a_{33} \cdot \Theta_v$$

$$\text{where } a_{32} = \frac{2D_4}{v_v \cdot \rho_v \cdot c_c}; a_{33} = \frac{2D_2}{v_v \cdot \rho_v \cdot c_c}.$$

Thus, in general, the mathematical model of the process of benzene alkyd is propylene in the liquid phase as follows:

$$\left. \begin{aligned} \frac{\partial x_a}{dt} &= a_{11} \cdot x_a + a_{12} \cdot \Theta \\ \frac{\partial \Theta}{dt} &= b_2 \cdot F_p + a_{22} \cdot \Theta + a_{21} \cdot x_a + a_{23}(\Theta_{v1} + \Theta_v) \\ \frac{\partial \Theta_v}{dt} &= a_{32} \cdot \Theta + a_{33} \cdot \Theta_v \end{aligned} \right\}$$

The task of synthesis of optimum linear regulator is solved. Based on the resolution of the matrix differential equation of the Rikatti and finding the optimum control. The Rikatti equation was resolved in reverse time.

The matrix differential equation of Rikatti is described by the formula:

$$P' = -PA - A^T P + PBR^{-1}B^T P - Q.$$

Where:

A – variable status matrix; B – management matrix; Q, R – matrix of weight coefficients from the:

$$A = \begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \end{pmatrix} \quad B = \begin{pmatrix} 0 \\ b_2 \\ 0 \end{pmatrix} \quad Q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, R=1.$$

We will write in the form of:

$$\begin{aligned} & \begin{pmatrix} P'_{11} & P'_{12} & P'_{13} \\ P'_{21} & P'_{22} & P'_{23} \\ P'_{31} & P'_{32} & P'_{33} \end{pmatrix} = - \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & 0 \\ a_{21} & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \end{pmatrix} - \begin{pmatrix} a_{11} & a_{21} & 0 \\ a_{12} & a_{22} & a_{32} \\ 0 & a_{23} & a_{33} \end{pmatrix} \times \\ & \times \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} + \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} 0 \\ b_2 \\ 0 \end{pmatrix} r^{-1} (0 \quad b_2 \quad 0) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} - \\ & - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}; r=1 \end{aligned}$$

$$\begin{aligned}
 P'_{11} &= -2a_{11}P_{11} - 2a_{21}P_{12} + b_2^2 P_{12}^2 - 1, \\
 P'_{12} &= P'_{21} = -a_{21}P_{12}^2 - a_{12}P_{11} - a_{22}P_{12} - a_{32}P_{13} + b_2^2 P_{12}^2, \\
 P'_{13} &= P'_{31} = -(a_{33} + a_{11})P_{13} - a_{23}P_{12} - a_{21}P_{23} + b_2^2 P_{12}P_{23}, \\
 P'_{22} &= -2a_{22}P_{22} - 2a_{12}P_{12} - 2a_{32}P_{23} + b_2^2 P_{22}^2 - 1, \\
 P'_{23} &= P'_{32} = -(a_{33} + a_{22})P_{23} - a_{23}P_{22} - a_{12}P_{13} - a_{33}P_{33} + b_2^2 P_{23}P_{22}, \\
 P'_{33} &= -2a_{33}P_{33} - 2a_{23}P_{23} + b_2^2 P_{13}P_{32}.
 \end{aligned}$$

Transversatnosti conditions:

$$P_{11}(t_f) = 0; P_{12}(t_f) = 0; P_{13}(t_f) = 0; P_{22}(t_f) = 0; P_{23}(t_f) = 0; P_{33}(t_f) = 0.$$

Optimum control equals:

$$\begin{aligned}
 \Delta U^*(t) &= -R^{-1} B^T P X = -R^{-1} \begin{pmatrix} 0 & b_2 & 0 \end{pmatrix} \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \\
 &= -r^{-1} b_2 (P_{12} \cdot \Delta x_1 + P_{22} \cdot \Delta x_2 + P_{23} \cdot \Delta x_3)
 \end{aligned}$$

The mathematical model of the process dynamics of benzene alkylation is developed in liquid phase. Chosen optimality criterion of the system. This approach allowed to synthesize the optimal linear law on the basis of application of matrix differential equation Rikatti. Found optimum control process of benzene alkyd propylene in liquid phase.

REFERENCE

1. YUKELSON I.I.: Technology of Basic Organic Synthesis "Text": Study. benefit I. I. Yukelson; Under Ed. Uryvalova NI - M.: Chemistry, 1968.
2. KLUSTA T.: Alkylator as the technology object [text]/T. Klusta, Z. Kozanevych//V Mizhnar. Sciences.-Prkt. Conf. Young scientists, postgraduates and stud. (AKIT – 2018), Kyiv, 11 – 12 Apr 2018 P.-Kyiv: KPI them. Igor Sikorsky, "Politekhnik", 2018. – 168 p. – ISBN 978-966-622-884-3
3. KLUSTA T.: Research of dynamic characteristics of alkylator benzene [text]/T. Klusta, Z. Kozanevych//Automation and computer-integrated technologies [text]: Abstracts of reports of twelfth scientific-practical conference of students. Kyiv, KPI them. Igor Sikorsky, 05 – 06 December 2018, [electronic resource]. Access mode: <http://ahv.kpi.ua/conferences/ACIT-2018> (Winter). pdf
4. LADIEVA L.: Optimization of technological processes.-K.: NMVO, 2003.
5. LADIEVA L. Optimal control systems.: Training manual.-K.: NMVO, 2000.