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STUDY OF THE FEATURES OF MONITORING THE RECTIFICATION PROCESS DURING AUTOMATIC CONTROL USING MOBILE INFLUENCES

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ABSTRACT

Aim of the research was to study sensitivity to disturbances of contact devices of rectification column at different values of mobile control actions and to determine specific of changes in a number of control tray when changing feed input point. Temperature profiles were calculated for rectification column for separation of methyl tret-butyl ether (MTBE) synthesis product at different values of main process disturbance of feed flow rate. It was found that there is the region with the highest and lowest sensitivity within the apparatus, which allows for control over the process in one or few points. The reaction of each tray to disturbances in feed flow rate was studied and a number of control contact device was found based on average sensitivity. It was discovered, that when mobile control approach is used, the control point of the rectification column with the highest sensitivity to disturbances is also mobile. A dependency of control contact device number of the column on value of mobile control action was found, which lies in changes of the column's feed input point.

Keywords: multicomponent rectification, mobile control, MTBE, sensitivity, temperature profile, mathematical modeling.

1. INTRODUCTION

Rectification - one of the main processes in chemical, oil, food and other industrial fields [1]. It enables separation of homogeneous liquid mixtures into their components. It is based on heat and mass transfer between the liquid and vapor phases on each contact devices of special column-type apparatus.

In terms of automatic control, the rectification column is a multivariable distributed object with significant delay times in controlling valves [2].

A feature of an object with distributed parameters is that their main parameters have the character of dimensional fields [3]. Information on parameter values at each point of the field is excessive and unequal. Thus measurements are recorded by sensors situated in one or more point of the dimension. There are also control points, at which parameter measurements would allow for improvement in the control system, compared to any other variants of object monitoring [4].

The problem of control is complicated by the necessity of using distributed or mobile control action when controlling dimensional fields. Control systems should provide best mass transfer conditions on each contact devices of the column at each moment in time, which is achievable through actions at intermediate points of rectification apparatus, which have distributed character in dimension and time [5]. Change of control action point and process conditions results in rational control point ales being mobile inside the column dimension.

The problem of mobile control involves a set of connected problems regarding the choice of a mathematical model of the process; parameters that can be controlled and regulated; method of mobile control and organization of rational information gathering under different process conditions and different control points [6].

The mathematical model should account for mobile control actions, distribution of rectification column as control objected and allow for calculations of process parameters in each point. Calculations assume determination of parameters in liquid and vapor phase on each tray of the column, including reboiler and condenser, using "stage-to-stage" method [7]. Mathematical model of contact device [8] includes equations of total and component material balances, heat balance equation, phase equilibrium model and calculation of efficiency coefficient of mass transfer at the tray. Problems of choosing calculation method [9] and static optimization [10] of the rectification process were solved including mobile control actions.

Majority of published works use change in reflux and heat agent flows as control actions for the process [11,

12]. In this case, influence points are located at ends of apparatus, which does not allow for optimal characteristics across the whole height of the rectification column.

The solution to this situation is to employ control actions by changing feed input or redistribution of this flow between the contact device in different parts. Such an approach allows influencing concentration and temperature profile of rectification apparatus [13 - 15].

Relocation of compound feed and energy over the column's height should be conducted in response to disturbances in the process. The main ones lie in changes in feed flow: flow rate, composition, and temperature [16]. Real-time measurements of disturbances are difficult, which leads to the use of regime process parameters [17]. Changes in flow rate or feed compositions lead to changes in material and energy load of the column, resulting in changes in the temperature profile of the apparatus. However, each contact device of the columns reacts differently to the same disturbance, with force and character of such reaction being determined by the value of mobile control action.

As such, in direction of mobile control and rectification control process the problems of parametric object analysis, the reasoning of control and regulation parameter and main process disturbances are solved; choice of solution method and static process optimization with the use of mobile control. The question of choosing rational control point at changes of intensity and coordinates of influences on the process is still open.

2. MATERIALS AND METHODS

The rectification process is subject to the influence of external disturbances, the main of which are changes in feed flow characteristics. Influence of such disturbances on static characteristics of the rectification column should be studied first. The present work is limited to external influence from the feed flow rate.

Study was conducted with use of mathematical model of multicomponent rectification process, adapted for solving problems of mobile control, and contains:

a) Contact device model

$$L_j + V_j = L_{j+1} + V_{j-1} + F_j; \quad (1)$$

$$L_j \cdot \bar{x}_j + V_j \cdot \bar{y}_j = L_{j+1} \cdot \bar{x}_{j+1} + V_{j-1} \cdot \bar{y}_{j-1} + F_j \cdot \bar{x}_{f,j}; \quad (2)$$

$$Q_{f,j} = F_j \cdot (z_j \cdot h_{F,j} + (1 - z_j) \cdot H_{F,j}); \quad (3)$$

$$L_j \cdot h_j + V_j \cdot H_j = L_{j+1} \cdot h_{j+1} + V_{j-1} \cdot H_{j-1} + Q_{f,j}; \quad (4)$$

$$h_{j+1} = f(\bar{x}_{j+1}, P_j); \quad (5)$$

$$H_j = f(\bar{y}_j, P_j); \quad (6)$$

$$h_{F,j} = f(\bar{x}_{F,j}, P_{f,j}, t_{f,j}); \quad (7)$$

$$H_{F,j} = f(\bar{y}_{F,j}, P_{f,j}, t_{f,j}); \quad (8)$$

$$\bar{y}_j^* = f(\bar{x}_j, P_j); \quad (9)$$

$$y_{j,i} = y_{j-1,i} + (y_{j,i}^* - y_{j-1,i}) \cdot \eta_{j,i}; \quad (10)$$

$$\sum_{i=1}^{n} x_{j,i} = \sum_{i=1}^{n} y_{j,i} = 1; \quad (11)$$

$$\begin{cases} F_j = q \cdot F, & j = N_{f,1}, \\ F_j = (1-q) \cdot F, & j = N_{f,2}, \\ F_j = 0, & j \neq N_{f,1}, \neq N_{f,2}, \end{cases} \quad (12)$$

where F - molar feed flow, kmol./h; h - liquid phase enthalpy, kJ/kmol.; H - vapor phase enthalpy, kJ/kmol.; L - molar feed flow of liquid phase, kmol./h; n - number of component in feed; P - pressure, MPa; Q - heat flow, kJ/h; V - molar feed flow of vapor phase, kmol/h; x - molar concentration of component in liquid phase, kmol/ kmol; y - molar concentration of component in vapor phase, kmol./kmol.; z - part of liquid phase in feed; η - Murphree efficiency of column's contact device. Lower indexes: F - parameter of liquid or vapor phase of feed; f - feed parameter; i - reviewed mixture component; j - number of column's contact device. Upper index: * - equilibrium parameter.

To account for mobile control actions, following independent variables were added to process model: $N_{f,1}$ - number of the feed tray, $N_{f,2}$ - number of the second tray during feed redistribution; q – feed redistribution coefficient.

When calculating trays from bottom to top, the defining parameters are characteristics of flows above the tray; a mirror problem when calculating the contact device from top to bottom.

Column's thermal profile is determined by boiling temperatures of liquid phases on its contact devices and is a function from compositions of given mixture and pressure on each tray. Concentration profiles are calculated according to (1) - (12).

Temperatures are calculated using method of solution theory using Antoine and NRTL equations [18]. The later allows to account for intermolecular interactions in liquid mixture and deviation from ideal related to it.

$$y_i^* = \frac{P_i}{P} \cdot \gamma_i \cdot x_i; \quad (13)$$

$$\ln P_i = C_{1i} + \frac{C_{2i}}{C_{3i} + T_{boil}} + C_{4i} \cdot \ln(T_{boil}) + C_{5i} \cdot T_{boil}^{C_{6i}}; \quad (14)$$

$$\ln\gamma_i = \frac{\sum_{j=1}^{n} x_j \cdot \tau_{ji} \cdot G_{ji}}{\sum_{k=1}^{v} x_k \cdot G_{ki}} + \sum_{j=1}^{n} \frac{x_j \cdot G_{ij}}{\sum_{k=1}^{n} x_k \cdot G_{kj}} \cdot \left(\tau_{ij} - \frac{\sum_{m=1}^{n} x_m \cdot \tau_{mj} \cdot G_{mj}}{\sum_{k=1}^{n} x_k \cdot G_{kj}} \right); \quad (15)$$

$$G_{ij} = e^{\left(-\alpha_{ij} \cdot \tau_{ij}\right)}; \quad (16)$$

$$\tau_{ij} = \frac{A_{ij}}{R \cdot T_{boil}}; \quad (17)$$

$$\tau_{ii} = \tau_{jj} = 0; \quad (18)$$

$$G_{ii} = G_{jj} = 1, \quad (19)$$

where A - parameter of approximated equation; C - empirical coefficient of Antoine equation; G - parameter of interaction between components i and j; R - universal gas constant, kJ/(kmol.·K); T - temperature, K; α, τ - independent parameters of binary interactions of NRTL equation; γ - activity coefficient. Lower indexes: ii, jj - numbers of binary system components; $boil$ – parameter determining boiling conditions.

Enthalpies of liquid and vapor phases are calculated with account for mixing heat of liquid mixture components

$$h = \sum_{i=1}^{n} \left(x_i \cdot \int_0^t c_{x,i}(t) dt \right) - R \cdot T^2 \cdot \sum_{i=1}^{n} \left(\frac{\partial \ln \gamma_i}{\partial T} \cdot x_i \right); \quad (20)$$

$$H = \sum_{i=1}^{n} \left(y_i \cdot \left(\int_0^{t_{boil}} c_{x,i}(t) dt + r_i + \int_{t_{boil}}^{t} c_{y,i}(t) dt \right) \right). \quad (21)$$

where c - molar heat capacity at constant pressure, kJ/(kmol.·K); r - molar heat of vaporization, kJ/kmol..; t - temperature, °C. Lower indexes: x - liquid phase parameter; y - vapor phase parameter.

b) Model reboiler

$$L_1 = V_0 + W; \quad (22)$$

$$L_1 \cdot \bar{x}_1 = V_0 \cdot \bar{y}_0 + W \cdot \bar{x}_w; \quad (23)$$

$$Q_w + L_1 \cdot h_1 = V_0 \cdot H_0 + W \cdot h_w; \quad (24)$$

$$h_w = f(\bar{x}_w, P_w); \quad (25)$$

$$H_0 = f(\bar{y}_0, P_w); \quad (26)$$

$$h_1 = f(\bar{x}_1, P_w); \quad (27)$$

$$\bar{y}_0^* = f(\bar{x}_w, P_w); \quad (28)$$

$$y_{0,i} = x_{w,i} + (y_{0,i}^* - x_{w,i}) \cdot \eta_{0,i}; \quad (29)$$

$$\sum_{i=1}^{n} x_{j,i} = \sum_{i=1}^{n} y_{j,i} = 1. \quad (30)$$

where W - molar flow of bottom product, kmol./h; Lower indexes: w, 0 - parameter of bottom product, reboiler.

c) Condenser model

$$Fl = V_N - D; \quad (31)$$

$$\bar{y}_{N+1}^* = f(\bar{x}_{fl}, P_d); \quad (32)$$

$$x_{d,i} = y_{N,i} + (y_{N+1,i}^* - y_{N,i}) \cdot \eta_{N+1,i}; \quad (33)$$

$$h_d = f(\bar{x}_d, P_d, t_d); \quad (34)$$

$$Q_d = Fl \cdot h_{fl} + D \cdot h_d - V_N \cdot H_N; \quad (35)$$

$$\sum_{i=1}^{n} x_{j,i} = \sum_{i=1}^{n} y_{j,i} = 1. \quad (36)$$

where D - molar flow of distillate, kmol./h; Fl - molar flow of reflux, kmol./h. Lower indexes: d, N+2 - distillate parameter; fl, N+1 - parameter of reflux, condenser.

d) equations of material and heat balances of rectification column

$$D = F - W; \quad (37)$$

$$x_{d,i} = \frac{F \cdot x_{f,i} - W \cdot x_{w,i}}{F - W}; \quad (38)$$

$$Q_d = W \cdot h_w + D \cdot h_d - F \cdot h_f - Q_w. \quad (39)$$

Boling temperatures of liquid mixtures are found by means of simple iterations for system of nonlinear equations (11), (13) - (19). Iterative calculations of rectification column's contact device, reboiler and condenser are conducted by means of interpolation. Modified θ-method is used to determine static characteristics of the process.

Study was conducted by means of mathematical modeling of rectification column for separation products of methyl tret-butyl ether (MTBE), which is used as additive to gasoline to increase octane number [19]. Column has 51 trays, external reboiler and condenser. 10 main component of feed were considered: propane (0.0098 mol. part), n-butane (0.077), isobutane (0.5346), butylene (0.0865), cis-butene (0.0394), trans-butene (0.0682), isobutylene (0.0044), pentane (0.00598), methanol (0.0421) and MTBE (0.132).

Initial parameters defining standard operation of apparatus: F=63.94 kmol./h; W=5.93 kmol./h; Q_w=2.395 GJ/h; P_w=5.2 kgs/cm^2, P_d=3.9 kgs/cm^2, P_f=9.3 kgs/cm^2, N_f=34. Feed, reflux and distillate are in liquid phase at boiling temperature. Following efficiency values were used for contact devices η: for trays 1 to 8 - 0.143; 9 to 51 - 0.096.

Defining parameters are flows rates of vapor and liquid phases at each cross-section of apparatus, concentration and temperature profiles of the column, energy load of condenser. Combination of input variable for the model includes main process disturbances - flow rate, composition and energy state of the feed and traditional control actions - heat load of reboiler, flow rate of the reflux. Change of tray number is considered as mobile control action

$$\overline{L},\overline{V},\overline{x_i},\overline{y_i},\overline{t},Q_d = f\left(N_f,Q_w,D,F,\overline{x_f},t_f,P_f,\overline{P},t_{fl},t_d,\overline{\eta_i}\right) \quad (40)$$

Tray's sensitivity to disturbance is determined by the ratio of temperature change on the contact device to flow rate change that caused it

$$S_j(F) = \frac{\Delta t_j(F)}{\Delta F} = \frac{t_j(F) - t_{j,n}(F_n)}{F - F_n}. \quad (41)$$

Calculation of the control tray number was conducted via scanning method. Additionally, the average sensitivity of each contact device $\overline{S_j}$ was calculated over the whole range of feed flow rate changes and number tray that is most sensitive to disturbance was found

$$\overline{S_j} = \frac{1}{F_h - F_l} \cdot \int_{F_l}^{F_h} S_j(F)dF. \quad (42)$$

3. RESULTS AND DISCUSSIONS

Temperature profile of rectification column (Figure-1) were calculated for its standard operation regime (F=F_n=63.94 kmol//h), and at 20% positive (F_h=76.73 kmol./h) and negative (F_l=51.15 kmol./h) disturbances of feed flow rate.

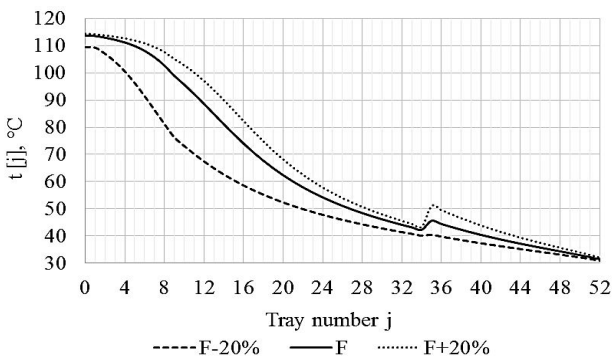

Figure-1. Temperature profiles of rectification columns at different feed flow rates.

Temperature changes were calculated at each contact device of the column for given disturbances relative to standard operation regime (Figure-2).

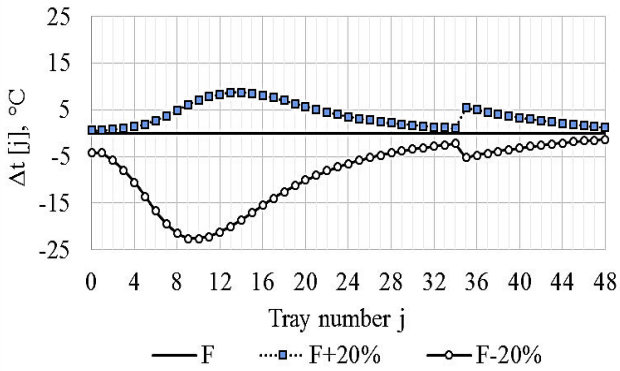

Figure-2. Changes in temperature profile at disturbances in feed flow rates.

As seen from Figure-1 and Figure-2, the region with the highest sensitivity are located in the lower part of apparatus, and distillate temperature is almost independent of feed flow rate. Increasing load of column results in increased temperature at all contact devices. The situation is revered for lowered feed flow rate. Lowering the material and energy load of column results in a stronger reaction from the rectification column than increase.

When feed is supplied to regulated tray 34, the biggest temperature deviation for negative disturbance is observed at contact device 10 and is -22.63°C. With equal positive of - 8.71°C on tray 14s.

The maximum for this value is 1.77°C·h/kmol. when the feed flow rate is lowered by 20% and 0.68°C·h/kmol. for the analogous increase. As such, sensitivity to disturbances of each contact device of the column depends on the value of disturbance. The dependency data for trays 10, 12 and 14 are shown in Figure-3.

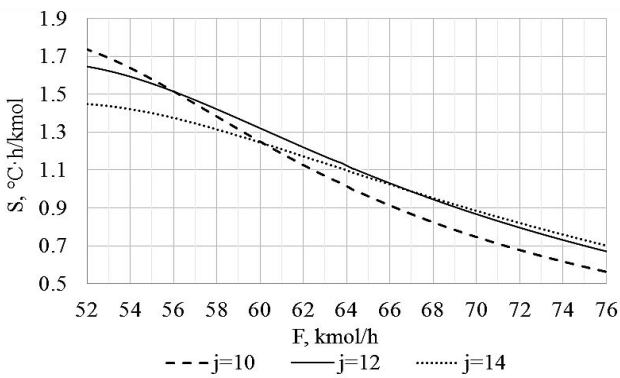

Figure-3. The sensitivity of the column's contact devices to disturbances in feed flow rate.

The calculation results of medium sensitivity (42) are shown in the Table-1.

Table-1. The average sensitivity of the column's contact devices to disturbances in feed flow rate.

j	5	6	7	8	9	10	11
$\overline{S}_j$, °C·h/kmol	0.412	0.546	0.701	0.861	1.008	1.083	1.131
j	12	13	14	15	16	17	18
$\overline{S}_j$, °C·h/kmol	1.149	1.137	1.097	1.037	0.963	0.882	0.799

As such, the tray 12 is controlled contact device of the column, with a maximum average sensitivity of 1.149 °C·h/kmol.

Conducted calculate and conclusions obtained for regulated column input when feed is supplied to tray 35. There is still a question of location for control point of apparatus at different values of mobile control action of the process.

Trays from 24 to 44 were assumed as feed tray and calculations were conducted for a contact device that is most sensitive to disturbances N_k (Figures 4, 5).

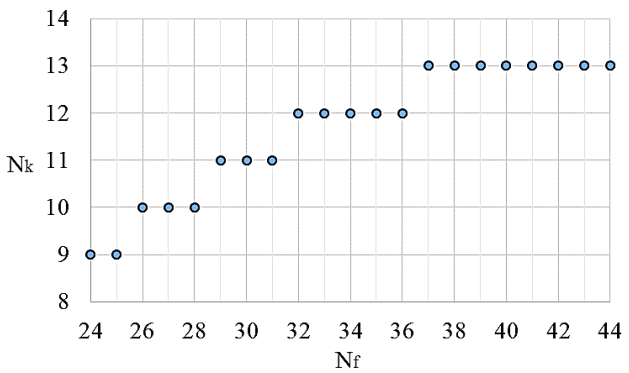

Figure-4. The dependence of the column's control contact device on the value of mobile control action - number of the feed tray.

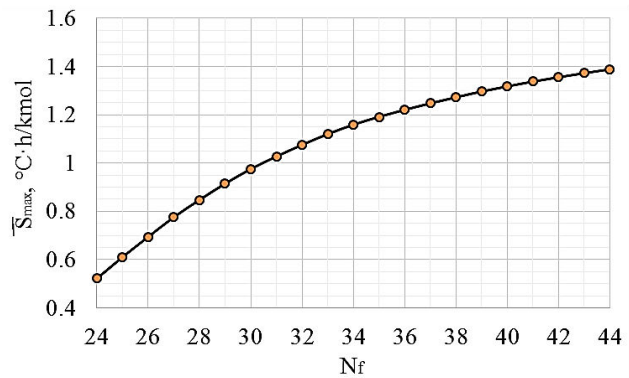

Figure-5. Average sensitivities of control contact devices of the column at different values of mobile control action.

Rectification column control point with the highest sensitivity to disturbances is also a mobile value. However, as seen from Figure-4, at the significant change of feed input point of the column by 20 contact devices, a number of control contact tray is shifted by 4 contact devices. This corresponds to the shift in a number of control tray at changes in the value of most disturbing action.

When the input point is moved upwards, a number of control contact device also increases. The average seniti to disturbances also increases: the higher the feed tray, the higher the change of parameters on the control tray in response to disturbance of the same intensity.

It should also be noted, that chaise of specific contact device as control must be done with account for the dynamic characteristic of «feed flow rate - temperature» and «feed composition - temperature» channels.

4. CONCLUSIONS

Temperature profiles were calculated for rectification column for separation of MTBE synthesis product at different values of main process disturbance of feed flow rate. Results revealed the existence of regions with the highest sensitivity to disturbances within the apparatus, which are primarily located in the lower part of the apparatus and include contact devices with numbers from 9 to 14.

The reaction of each tray to disturbances in the feed flow rate was studied. The biggest temperature deviation for negative disturbance is observed at contact device 10 and is -22.63°C. With equal positive of - 8.71°C on tray 14s.

A number of most sensitive control tray of the column was found, based on the average sensitive of contact devices to disturbances. In this case tray, 12 must be used, which has a maximum average sensitivity of 1.149 °C·h/kmol.

A dependency of control contact device number of the column on value of mobile control action was found, which lies in changes of the column's feed input point. When feed is supplied onto trays 24 and 25, temperature control should be realized on contact device 9, 26 and 28 - 10, 29 and 31 - 11, 32 and 36 - 12, 37 and 44 - 13.

It was found that for the studied column the increasing number of feed tray increase average sensitivity of control contact device. When feed is supplied to tray 24, the average sensitivity of the control contact device is 0.52°C·h/kmol.; at supply to tray 44 - 1.39°C·h/kmol.

Results of conducted steed are applicable to the construction of mobile control systems for controlling rectification processes with mobile control, adaptive,

optimal pressure systems. Further study in this direction like in the study of dynamic characteristics of the process in channels «disturbance - the temperature at control contact devicee» with account for delay time. The sensitivity of contact devices of rectification apparatus to disturbances from composition and temperature of feed at different values of mobile control actions are also subject of analysis.

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