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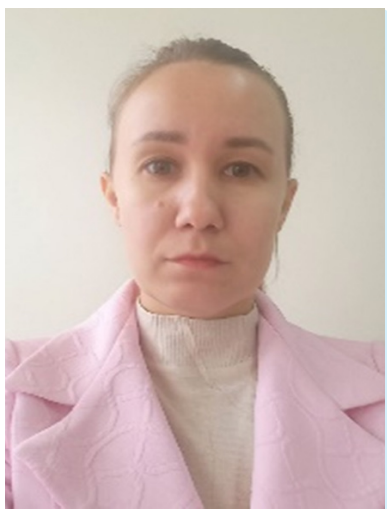
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DEVELOPMENT OF A MIMO MODEL OF AZEOTROPIC DISTILLATION

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Abstract: The article addresses the development of a dynamic MIMO model of the azeotropic distillation process as an object of automatic control. The process is characterized by strong multivariable interactions, nonlinearity, and the presence of vapor–liquid equilibrium involving an entrainer. Based on a simplified MESH approach, a state-space matrix model suitable for dynamic analysis and the synthesis of predictive controllers is obtained. A structural diagram of the azeotropic distillation column and transient responses of the main control channels are presented.

Key words: azeotropic distillation, MIMO model, dynamic model, heat and mass transfer, entrainer, control system, transient responses.

Annotatsiya: Maqolada azeotropik rektifikatsiya jarayonining avtomatik boshqaruv obyekti sifatida dinamik MIMO–modelini qurish masalalari ko'rib chiqilgan. Jarayon kuchli o'zaro bog'liqlik, nolinearlik hamda entrayner ishtirokidagi fazaviy muvozanatning mavjudligi bilan tavsiflanadi. Soddalashtirilgan MESH yondashuvi asosida dinamika tahlili va prediktiv regulyatorlarni sintez qilish vazifalari uchun mos bo'lgan holatlarning matritsali modeli olingan. Azeotropik rektifikatsiya kolonkasining strukturaviy sxemasi hamda boshqaruvning asosiy kanallari bo'yicha o'tish xarakteristikalarini keltirilgan.

Kalit so'zlar: azeotropik rektifikatsiya, MIMO–model, dinamik model, issiqlik va massa almashinuvi, entrayner, boshqaruv tizimi, o'tish xarakteristikalarini.

Аннотация: В статье рассматривается построение динамической MIMO–модели процесса азеотропной ректификации как объекта автоматического управления. Процесс характеризуется сильной многосвязностью, нелинейностью и наличием фазового равновесия с участием энтрейнера. На основе упрощённого MESH–подхода получена матричная модель состояния, пригодная для задач анализа динамики и синтеза предиктивных регуляторов. Представлены структурная схема азеотропной ректификационной колонны и переходные характеристики по основным каналам управления.

Ключевые слова: азеотропная ректификация, MIMO–модель, динамическая модель, тепломассообмен, энтрейнер, система управления, переходные характеристики.

INTRODUCTION

Azeotropic distillation is widely used in the chemical, petrochemical, and food industries for the separation of mixtures that cannot be separated by conventional binary distillation. Typical applications include the production of absolute ethanol, dehydration of organic solvents, and separation of close-boiling components.

From the viewpoint of automatic control, the azeotropic distillation process belongs to the class of complex multivariable (MIMO) systems, which are characterized by strong cross-coupling between control channels,

significant time delays and inertia, nonlinearity of phase equilibrium, and the influence of the entrainer and decanter on system dynamics.

Therefore, the development of an adequate MIMO model that provides a basis for dynamic analysis and the design of advanced control algorithms, including Model Predictive Control (MPC), is a relevant and practically important task.

REVIEW OF LITERATURE ON THE SUBJECT

Azeotropic distillation is one of the most complex heat- and mass-transfer processes, requiring consideration of liquid-phase non-ideality, multivariable dynamics, and phase separation in the overhead system. For ethanol–water systems, conventional distillation is limited by the existence of an azeotropic point, which necessitates the use of entrainers and decanters and significantly complicates both modeling and control.

Recent studies on azeotropic and extractive distillation rely on thermodynamic activity-coefficient models such as NRTL, UNIQUAC, and Wilson, which enable accurate description of VLE/LLE behavior in the presence of an entrainer. These models are discussed in detail in works devoted to advanced distillation technologies and conceptual design of complex column configurations, emphasizing the crucial role of the overhead “condenser–decanter–reflux” loop in determining system dynamics [1–4].

Dynamic modeling of distillation columns in recent years is predominantly based on the MESH approach, which provides a reasonable compromise between model accuracy and computational complexity. Despite the development of rate-based models, linearized models obtained around steady-state operating points with subsequent order reduction are more commonly used for dynamic analysis and control synthesis [2,5]. This approach is especially relevant for azeotropic distillation, where the full model dimension may reach several tens of states.

In the field of distillation control, significant attention is paid to the MIMO representation of the process, since changes in reflux flow rate, reboiler heat duty, and entrainer flow rate lead to substantial cross-effects on distillate composition, bottom composition, and temperature profiles. For practical purposes, first- and second-order plus dead-time (FOPDT/SOPDT) transfer-function matrices and state-space models are widely employed [5–7].

Multivariable interaction analysis is traditionally performed using the Relative Gain Array (RGA) and related frequency- and steady-state criteria, which justify the necessity of multivariable control and proper input–output pairing [7]. It has been shown that SISO-based approaches applied to azeotropic columns often result in degraded dynamic performance and increased oscillations.

Over the past 15 years, the application of Model Predictive Control to distillation processes, including azeotropic configurations, has developed intensively. MPC accounts for multivariable interactions, time delays, and operational constraints, which is particularly important for entrainer flow rate and thermal load control. Several studies highlight the effectiveness of linear MPC based on MIMO models obtained through step-response identification or linearization of detailed nonlinear models [6–8].

Thus, analysis of modern publications indicates that the development of an adequate MIMO model of azeotropic distillation is a necessary prerequisite for the synthesis of effective control systems. Despite significant progress in thermodynamic and dynamic modeling, issues related to structural identification, decanter dynamics, and cross-coupling effects remain relevant, defining the scientific novelty and practical significance of the present study.

RESEARCH METHODOLOGY

The objective of this study is the development and verification of a dynamic MIMO model of azeotropic distillation in the vicinity of a steady-state operating point, suitable for transient analysis and subsequent synthesis of multivariable control algorithms.

The object of study is a typical continuous azeotropic distillation unit comprising a column with N theoretical trays, a condenser, a reboiler, a decanter for distillate phase separation, feed streams of the binary mixture and the entrainer, and phase recycle loops [9–11]. Figure 1 shows the column with feed stream F , entrainer stream E , control inputs: reflux flow rate L , reboiler heat duty Q_R , condenser heat duty Q_C ; and output variables: distillate composition x_D , bottom composition x_B , and temperatures of selected trays T_i .

The process is assumed to operate at constant pressure, with the entrainer introduced into the upper section of the column.

The following assumptions are adopted: vapor–liquid equilibrium on each theoretical tray; constant pressure along the column height; pressure and liquid-level dynamics are neglected and assumed to be stabilized by lower-level control loops; local linearization of the model around a selected steady-state operating point (Figure 1).



Figure 1. Process flow diagram of an azeotropic distillation column

For the MIMO model, the following variables are selected.

Input variables (manipulated variables):

$$u(t) = [L(t) \quad Q_R(t) \quad E(t)]^T$$

where $L(t)$ is the reflux flow rate, $Q_R(t)$ is the reboiler heat duty, and $E(t)$ is the entrainer flow rate.

Output variables:

$$y(t) = [x_D(t) \quad x_B(t) \quad T_k(t)]^T,$$

where $x_D(t)$ is the mole fraction of the target component in the distillate, $x_B(t)$ is the mole fraction in the bottom product, and $T_k(t)$ is the temperature of a selected control tray.

Mathematical Description of the Process

In the development of the MIMO model, the distillation column is described by the MESH equations, where M denotes material balances, E phase-equilibrium relations, S steady-state vapor and liquid flow equations, and H energy balances.

For the i -th tray, the dynamic material balance is given by:

$$\frac{d(M_i x_i)}{dt} = L_{i+1} x_{i+1} + V_{i-1} y_{i-1} - L_i x_i - V_i y_i + F_i x_F,$$

where M_i is the liquid holdup on tray i , x_i , y_i – are mole fractions in the liquid and vapor phases, F_i represents external feeds (feed or entrainer), and x_F is their composition.

The energy balance for the i -th tray is:

$$\frac{d(M_i h_i)}{dt} = L_{i+1} h_{i+1} + V_{i-1} H_{i-1} - L_i h_i - V_i H_i + Q_i,$$

where h_i , H_i – are the specific enthalpies of the liquid and vapor phases, and Q_i represents heat flows and losses.

For azeotropic systems, phase equilibrium is described by the modified Raoult's law:

$$y_i = \gamma_i(T, x) \frac{P_i^{\text{вещ}}(T)}{P} x_i,$$

where γ_i is the activity coefficient calculated using models such as NRTL or UNIQUAC.

The resulting nonlinear system of differential equations serves as the basis for dynamic analysis and subsequent formation of a linearized MIMO model.

After linearization around the steady-state operating point, the following state-space representation is obtained:

$$\dot{x}(t) = Ax(t) + Bu(t),$$

$$y(t) = Cx(t),$$

where $x(t)$ is the state vector consisting of tray compositions and temperatures, and A , B , and C are the system, input, and output matrices, respectively.

The system dimension typically exceeds 20–50 states, confirming the multivariable nature of the process.

A classic example of azeotropic distillation is the ethanol–water system, for which a minimum-boiling azeotrope exists at atmospheric pressure at approximately 95.6 wt.% ethanol (≈ 0.895 mole fraction). Consequently, conventional distillation cannot exceed this concentration, and azeotropic distillation with an entrainer and a decanter is required. Cyclohexane or benzene is commonly used as an entrainer.

A compact six-state model is developed, where the states represent inertial dynamics of outputs and cross-coupling paths:

$$x(t) = [x_1, x_2, x_3, x_4, x_5, x_6]^T,$$

with x_1, x_2 – describing the dynamics of x_D ; x_3, x_4 – the dynamics of x_B ; x_5, x_6 – the dynamics of T_k .

Matrixes:

$$A = \begin{bmatrix} -1/60 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/45 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1/90 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1/70 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1/40 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1/35 \end{bmatrix}$$

$$B = \begin{bmatrix} -\frac{0.020}{60} & 0 & \frac{0.018}{60} \\ 0 & \frac{0.035}{45} & 0 \\ \frac{0.010}{90} & 0 & -\frac{0.012}{90} \\ 0 & -\frac{0.028}{70} & 0 \\ -\frac{1.20}{40} & 0 & \frac{0.90}{40} \\ 0 & \frac{2.10}{35} & 0 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

Each output is represented as a sum of two first-order dynamics, one corresponding to the dominant effect and the other to cross-coupling or thermal effects.

ANALYSIS AND RESULTS

To evaluate the dynamic properties of the MIMO object, transient responses were calculated for step changes in the manipulated variables (Figs. 2–4). The transient responses were obtained by applying step variations to each manipulated variable while keeping the remaining inputs constant. The Relative Gain Array (RGA) method was employed to analyze multivariable interactions and channel coupling, enabling a quantitative assessment of cross-effects between inputs and outputs. The proposed methodology provides a systematic transition from a detailed physicochemical description of azeotropic distillation to a compact MIMO model suitable for dynamic analysis, multivariable interaction assessment, and subsequent synthesis of predictive control algorithms (Figure 2; 3; 4) [12].

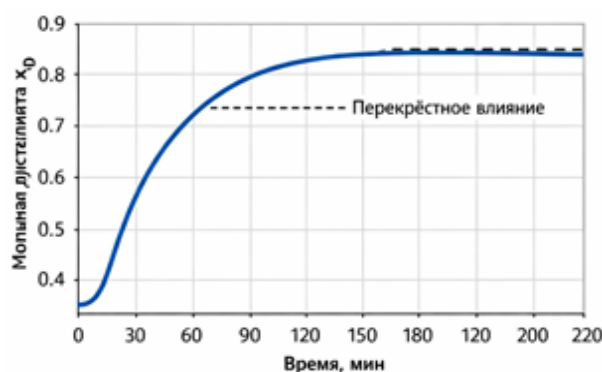


Figure 2. Transient response of the $L \rightarrow x_D$ channel

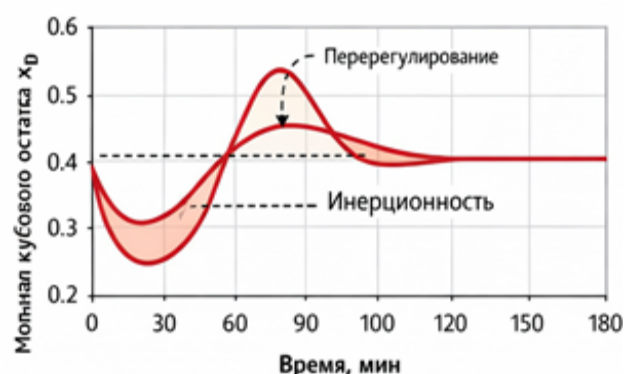


Figure 3. Transient response of the $QR \rightarrow x_B$ channel

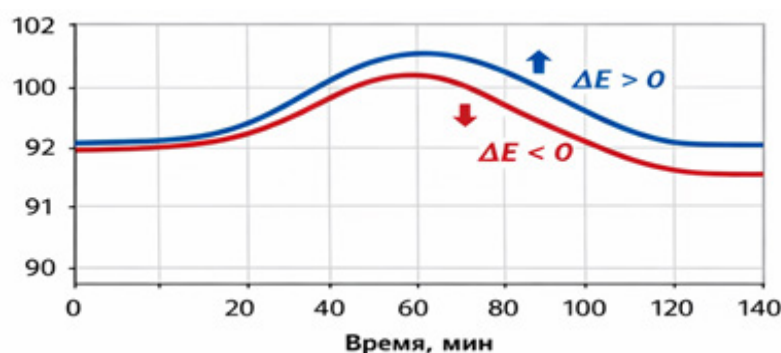


Figure 4. Cross-effect of the $E \rightarrow T_k$ channel

The $L \rightarrow x_D$ channel exhibits an aperiodic response with a long settling time and a pronounced influence of cross-coupling effects.

The $Q_R \rightarrow x_B$ channel demonstrates inertial behavior with overshoot caused by the thermal capacitance of the reboiler.

The $E \rightarrow T_k$ channel indicates that variations in the entrainer flow rate significantly affect the temperature profile of the column.

The developed MIMO model enables quantitative evaluation of the degree of multivariable coupling, identification of dominant dynamic interactions, use of the model as a basis for MPC algorithm synthesis, and execution of virtual experiments without direct intervention in the real process. It should be noted that simplification of the MESH model reduces computational complexity while preserving the key dynamic characteristics of the process.

CONCLUSIONS AND SUGGESTIONS

A dynamic MIMO model of azeotropic distillation based on material and energy balances with phase-equilibrium considerations has been developed. The process is shown to be a strongly coupled and inertial control object. The presented transient responses confirm the necessity of multivariable control strategies for the operation of azeotropic distillation columns.

The obtained results can be used in the development of predictive control systems and digital twins of heat- and mass-transfer processes.

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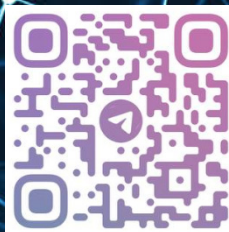
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