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ОПТИМАЛЬНОЕ УПРАВЛЕНИЕ СТАЦИОНАРНЫМИ РЕЖИМАМИ РЕКТИФИКАЦИОННОЙ КОЛОННЫ НА ОСНОВЕ НЕЛИНЕЙНОЙ МОДЕЛИ
OPTIMAL CONTROL OF STEADY-STATE REGIMES OF A RECTIFICATION COLUMN BASED ON A NONLINEAR MODEL

Аннотация. В исследовании задача оптимального управления стационарными режимами функционирования ректификационной колонны формулируется как оптимизация энергетического или экономического критерия при нелинейных ограничениях модели. Стационарное поведение колонны описывается материальными и компонентными балансами, соотношениями потока на тарелках, фазовым равновесием и энергетическими уравнениями, что приводит к многомерной нелинейной системе уравнений. В связи с сильной нелинейностью, вызванной зависимостью фазового равновесия от температуры и состава, предлагается аппроксимация этого блока с использованием нейронной сети в рамках гибридной модели. Для поддержания оптимального режима при наличии возмущений применяется механизм на основе скользящего режима в реальном масштабе времени. Такой подход позволяет отслеживать экстремумы без измерения производной целевой функции и повышает энергетическую и экономическую эффективность работы колонны.

Abstract. In this study, the problem of optimal control of the steady-state operating modes of a distillation column is formulated as the optimization of an energy or economic criterion under nonlinear model constraints. The steady-state behavior of the column is described by material and component balances, tray flow relations, phase equilibrium, and energy equations, resulting in a high-dimensional nonlinear system of equations. Due to the strong nonlinearity caused by temperature–composition dependence in phase equilibrium, the approximation of this block using a neural network is proposed within a hybrid modeling framework. To maintain the optimal mode in the presence of disturbances, a mechanism based on a sliding mode in real time is used. This approach enables extremum tracking without measuring the derivative of the objective function and improves the energy and economic efficiency of the column's operation.

Ключевые слова: Ректификационная колонна, стационарный режим, нелинейная модель, нейронная сеть, управление скользящим режимом.

Keywords: Rectification column, steady-state regime, nonlinear model, neural network, sliding mode control.

Distillation columns are the principal units used for separation and purification in the chemical and petrochemical industries. Since the high degree of separation required in such columns is usually achieved through a significant reboiler heat duty, the optimal selection of operating conditions becomes a critical factor from the perspectives of both energy efficiency and economic performance. The steady-state representation of a distillation column is formed by the simultaneous solution of total and component material balances, tray-to-tray flow relations, phase equilibrium equations, and energy balance equations. Depending on the number of trays in the column, this structure leads to a high-dimensional system of coupled and nonlinear algebraic equations. The primary source of nonlinearity arises from phase equilibrium relationships. Consequently, steady-state optimization of the column essentially becomes a nonlinear constrained optimization problem in which the objective function must be optimized subject to these nonlinear relationships [1-8].

The objective of this study is to justify the optimal control of steady-state operating modes of a distillation column. As a result, a mathematical framework is proposed that enables both the computation of the optimal operating regime and its maintenance under disturbances, ensuring improved energy efficiency and economic performance. The problem of optimal control of the static operating modes of a distillation column can be formulated as the optimization of a nonlinear system of algebraic equations according to an economic or energy performance criterion. The steady-state behavior of the column is described through material balances, component balances, phase equilibrium relations, and energy balance equations.

The tray-by-tray material balance for the i-th stage of the column is written as

$$L_{i+1}x_{i+1} + V_{i-1}y_{i-1} + F_i z_i = L_i x_i + V_i y_i \quad (1)$$

When this system is written for all trays of the column, a high-dimensional nonlinear system of equations is obtained. Phase equilibrium in real systems exhibits nonlinear behavior due to the non-constant nature of relative volatility. In a simplified form, it can be represented as

$$y_i = \frac{\alpha x_i}{1+(\alpha-1)x_i} \quad (2)$$

However, in a more general formulation, the distribution coefficient is written as

$$y_i = K_i(T_i, P_i, x_i)\, x_i \quad (3)$$

where $K_i = \frac{\gamma_i(T_i,x_i)\, P_i^{sat}(T_i)}{P}$.

The functions γ_i and P_i^{sat} are strongly nonlinear. Therefore, approximating this part of the model using a neural network becomes an effective approach:

$$(x_i, T_i) = F_{NN}(y_i) \quad (4)$$

The neural network is represented in a two-layer feed-forward structure as follows:

$$h_j = \sigma_1\left(\sum_{i=1}^{n} w_{ji}^{(1)}\, x_i + w_{j0}^{(1)}\right) \quad (5)$$

$$y_k = \sigma_2\left(\sum_{j=1}^{p} w_{kj}^{(2)}\, h_j + w_{k0}^{(2)}\right) \quad (6)$$

The parameters of the network are determined by minimizing the error function:

$$E(w) = \frac{1}{2}\sum_{n=1}^{N} \| y(x^{(n)}, w) - \hat{y}^{(n)} \|^2 \quad (7)$$

This hybrid modeling approach allows the preservation of the physical structure of the distillation model while replacing the most computationally demanding nonlinear relationships with data-driven approximations.

The optimization update step using the gradient descent method is given by

$$w^{(\tau+1)} = w^{(\tau)} - \eta \nabla E(w^{(\tau)}) \quad (8)$$

Accordingly, the steady-state model of the column can be written in the general form:

$$F(x, u, F_{NN}(x)) = 0 \quad (9)$$

where x is the state variables (tray concentrations, temperatures), and u is the manipulated variables (reflux ratio, heat duty, etc.).

The reflux ratio is defined as

$$R = \frac{L_0}{D} \tag{10}$$

and the reboiler heat duty can be approximately expressed as

$$Q_{reb} \approx V_N \lambda \tag{11}$$

The objective function for minimizing energy consumption is taken as

$$J = Q_{reb} \tag{12}$$

or, in an economic formulation, as

$$\Pi = p_D D + p_B B - p_F F - p_E Q_{reb} \tag{13}$$

These expressions serve as the basis for formulating the optimization problem for the column's steady-state operation. The static optimization problem is formulated as:

$$\min_{x,u} J(x,u) \tag{14}$$

subject to the constraint $F(x,u,F_{NN}(x)) = 0$.

The Lagrange function is written as

$$L(x,u,\lambda) = J(x,u) + \lambda^T F(x,u,F_{NN}(x)) \tag{15}$$

and the necessary optimality conditions are given by

$$\nabla_x L = 0, \nabla_u L = 0, \quad F(x,u,F_{NN}(x)) = 0 \tag{16}$$

The Jacobian matrix

$$J_F = \frac{\partial F}{\partial x} \tag{17}$$

can be used to analyze the local stability of the system and the sensitivity of the solution. If the condition $\det(J_F) \neq 0$ is satisfied, then the steady-state point is locally unique. Therefore, the problem of optimal control of the static operating modes of a distillation column is essentially an optimization problem of a high-dimensional nonlinear algebraic system.

The optimization problem is formulated as

$$\min_{V} J(V) = -P(V) \tag{18}$$

The necessary condition for the optimal point is

$$\frac{dJ}{dV} = 0 \tag{19}$$

However, this criterion function is nonlinear in nature, and the extremum point shifts as the feed composition changes. Therefore, the function $V_{\text{opt}} = V_{\text{opt}}(z_F)$ is nonlinear, and classical fixed-parameter optimization approaches do not provide sufficiently reliable results. In this context, a Real-Time Optimization system based on sliding mode principles provides an alternative and more robust approach. In this method, the optimization problem is expressed as

$$J = -P(V), V = u \tag{20}$$

The sliding surfaces are defined as

$$\sigma_1 = \varepsilon, \sigma_2 = \varepsilon + \delta \tag{21}$$

where $\varepsilon = g - J$ and the reference signal dynamics are defined as

$$\frac{dg}{dt} = -\rho\sigma_1\sigma_2 + h(\sigma_1, \sigma_2) \tag{22}$$

The control law is chosen as

$$u = u_0 \operatorname{sign}(\sigma_1\sigma_2) \tag{23}$$

This mechanism ensures that the system moves toward the extremum direction without directly measuring the derivative of the objective function. In sliding mode, the system becomes less sensitive to uncertainties and parameter variations, ensuring stable convergence toward the optimal point. In this case, the condition must be satisfied:

$$\frac{\partial J}{\partial V} \cdot \frac{\partial V}{\partial u} \leq 0 \tag{24}$$

This condition ensures that the system enters the sliding regime and maintains stability. When the feed composition changes, the optimal boil-up value also shifts. However, the sliding mode mechanism automatically tracks this new optimal point, allowing the system to operate stably even under non-stationary conditions.

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