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# DEVELOPMENT OF A MODEL-BASED CONTROL ALGORITHM FOR AN AMMONIA SYNTHESIS COLUMN

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# РОЗРОБКА АЛГОРИТМУ МОДЕЛЬНО-ОРІЄНТОВАНОГО КЕРУВАННЯ КОЛОНОЮ СИНТЕЗУ АМІАКУ

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*This paper presents an approach to the development of a model-based control system for a multi-shelf synthesis column used in ammonia production. The proposed approach is based on the application of a combined mathematical model that integrates deterministic and experimental–statistical modeling methods. Such a combination makes it possible to achieve a high level of model adequacy, ensure adaptability to varying operating conditions, and expand the applicability of the model for the analysis and control of complex chemical engineering processes.*

*Using the proposed approach, a mathematical model of a three-shelf ammonia synthesis column equipped with an internal heat exchanger was developed. Based on this model, an information and logical scheme of the control object was refined, which made it possible to identify the key internal interactions between process variables and to assess their influence on the output parameters of the synthesis column. On this basis, an operating algorithm for a model-based control system was developed.*

*The obtained mathematical description enabled the formulation of an optimality criterion for column operation and the solution of an optimization problem aimed at determining the optimal flow rates of "cold" bypass streams. This makes it possible to maintain the operating conditions of the column in a region close to the optimal regime and to ensure a rapid transition of the system to this region during operation. The optimal value of ammonia concentration at the outlet of the synthesis column was determined using the Hooke–Jeeves optimization method.*

*A functional automation scheme was developed, and the set of technical means required for implementing the proposed control system in industrial automatic process control systems was analyzed. The implementation of the developed model-based control system will reduce deviations of technological parameters from their optimal values and improve the operational efficiency of the ammonia synthesis column.*

***Keywords:*** *ammonia production, synthesis column, model-based control, combined mathematical model, process optimization.*

**Introduction.** The continuous growth of raw material prices on global markets leads to a significant increase in production costs in the Ukrainian chemical industry. In particular, the share of natural gas in the total production cost at chemical enterprises currently reaches approximately 75%. Under such conditions, improving the efficiency of raw material and energy utilization becomes a key factor in ensuring the competitiveness of domestic products in the global market. Therefore, optimization of technological processes is an urgent task for modern chemical production.

Various approaches are used to improve the efficiency of industrial processes, including the development of new catalysts, modernization of technological equipment, and the implementation of automatic process control systems (APCS). However, for complex technological processes such as ammonia synthesis, where multi-shelf gas reactors are used, the simple replacement of local control systems with APCS does not ensure optimal process control.

At the same time, APCS provide the technological basis for implementing advanced model-based control systems for complex technological units, such as synthesis columns used in ammonia production. The primary objective of the reactor control system is to achieve the maximum conversion of the initial components of the reversible reaction by maintaining an optimal temperature profile along the reactor height. A characteristic feature of the synthesis process is that it is close to the ideal plug-flow model, which implies the existence of gradients of technological parameters along the spatial coordinate.

During the optimization of continuous large-scale chemical productions, such as ammonia synthesis, particular attention should be paid to the synthesis cycle, especially to the synthesis column. In such production processes, the synthesis column represents a sequence of interconnected gas reactors. Since synthesis reactions are typically exothermic, the heat released from the reaction is used to preheat the synthesis gas entering the column.

The temperature regime within the column is controlled by supplying synthesis gas through "cold" bypass streams that do not pass through the internal heat exchanger. These streams are introduced at the inlets of the corresponding shelves of the column. The main control problem for a multi-shelf synthesis column in ammonia production is the optimal distribution of synthesis gas flow through the physical channels of the column in order to maximize the concentration of the target component (ammonia) at the column outlet.

This problem can be solved by implementing a model-based control system. The development of such a system requires the creation of a mathematical model of the synthesis column and the design of an appropriate control algorithm. The mathematical model should be sufficiently simple to allow real-time implementation, while at the same time adequately reflecting the influence of numerous technological parameters. In addition, the model should be easily invertible, allowing the determination of the optimal flow rates of synthesis gas through the "cold" bypass streams on each column shelf based on the current value of the target component concentration.

However, the models presented in works [1, 2] do not meet these requirements and therefore cannot be directly applied for solving the considered control problem.

Taking into account the above considerations, the development of a mathematical model and an operating algorithm for a model-based control system of a multi-shelf ammonia synthesis column represents an urgent and important applied scientific problem.

Literature Data Analysis and Problem Statement

In paper [1], it was demonstrated that the parameters of a complex technological object such as a synthesis column are interconnected. A change in the synthesis gas flow through any of the "cold" bypass streams leads not only to a change in the temperature on the corresponding shelf but also affects the gas flow distribution through the physical channels of the column. Consequently, a change in the synthesis gas flow in any bypass pipeline influences the overall temperature regime of the column and, as a result, the concentration of the target component at the column outlet. However, the internal interconnections between the parameters were not sufficiently considered in the presented approach.

In study [2], it was shown that achieving maximum production efficiency requires an optimal distribution of synthesis gas flows through the physical channels of the synthesis column in such a way that the concentration of the target component at the column outlet is maximized. At the same time, the temperature at the shelves of the synthesis column must not exceed permissible technological limits. Therefore, the mathematical model must include corresponding constraints, which were not considered in the referenced work.

The specific features of the synthesis process were thoroughly analyzed in paper [3]. In [4], it was shown that the direct solution of the optimization problem is complicated due to the inherent properties of the control object, namely the large number of technological parameters. Variations in any of these parameters can shift the extremum of the concentration function, which significantly complicates the search for optimal operating conditions.

One possible approach to overcoming these difficulties is the use of model-based control systems [5]. A similar approach was proposed in [6], where a deterministic model was developed. In [7], the ideal plug-flow model with parameter gradients along the spatial coordinate was used. However, the practical application of this model is limited due to the complexity of identifying its parameters.

The analysis of studies [8], devoted to the development of static and dynamic models of synthesis columns and their internal heat exchangers, confirms the conclusions obtained. A critical analysis of existing approaches to modeling and control of synthesis columns makes it possible to formulate the research objective and define the main tasks of this study.

The aim of this study is to improve the operational efficiency of an ammonia synthesis column through the development of a model-based control system and an algorithm for searching optimal operating conditions.

To achieve this aim, the following research objectives are formulated:

– to analyze the ammonia synthesis process in a multi-shelf column as a control object;
– to develop static and dynamic mathematical models of the synthesis column;
– to design an algorithm for verifying the adequacy of the developed models and for determining the extreme value of the target component concentration at the outlet of the synthesis column (preliminary optimization stage);
– to implement a model-based control system and to investigate the performance of the proposed optimal control strategy for the synthesis column.

Materials and Methods for Studying the Information-Logical Structure of a Three-Shelf Ammonia Synthesis Column.

In this study, the parameters characterizing the state of the technological system are referred to as output parameters. The main objective of the control system is to maintain these parameters at their optimal values. Control parameters are variables through which the regulation process is carried out, such as material and energy flow rates. Disturbance parameters are variables that affect the output parameters but cannot be directly controlled.

An analysis of the technological process occurring in a three-shelf gas reactor used for ammonia synthesis (Fig. 1) shows that the object has two main output coordinates: the concentration of the target product $Q_3$at the column outlet and the gas temperature $T_3$at the column outlet after the heat exchanger $TO$.

For the considered object, the temperature distribution along the height of the ammonia synthesis column uniquely determines the ammonia concentration at the outlet and, consequently, the temperature $T_3$, which in turn determines the temperatures $T_0$and $T_3'$. Since the object can be considered, with sufficient accuracy, as a closed thermodynamic system, the concentration value $Q_3$uniquely determines the temperature $T_3$and, correspondingly, the temperatures $T_0$and $T_3'$. Therefore, stabilization of the temperature $T_3'$does not have independent practical significance in this case.

A specific feature of the considered object is that control of a single parameter—the concentration of the target component $Q_3$—is achieved using three control variables, namely the circulating gas flow rates supplied to each of the three catalyst shelves through cold bypass streams.

Disturbance parameters include the circulating gas flow rate $F_{c.g.}$, its temperature $T_{c.g.}$, and the concentration of the target component at the reactor inlet $Q_0$. The circulating gas pressure $P$can also be considered a disturbance parameter because it is stabilized by the synthesis gas compressor. Moreover, due to the relatively low conversion of synthesis gas into the final product (approximately 10%), the pressure drop caused by the reaction does not exceed about 5%. Therefore, when the conversion degree varies within the range of 8–12%, the pressure changes within 4–6%, which lies within the measurement error of the pressure control channel [4].

An information-logical analysis of the three-shelf ammonia synthesis column was carried out. Based on this analysis, a generalized information-logical scheme of a three-shelf ammonia synthesis column equipped with an internal recuperative heat exchanger was developed. The resulting scheme is presented in Fig. 1.

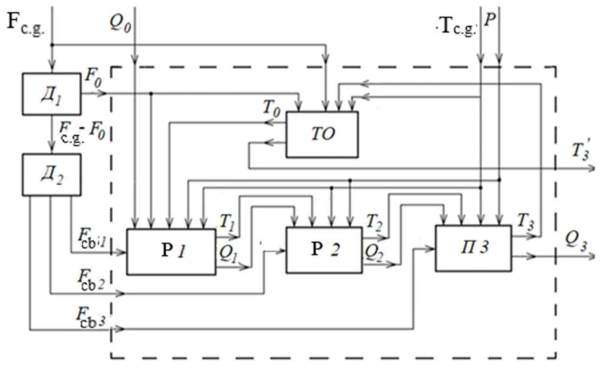


Fig. 1. Information-Logical Scheme
of a Three-Shelf Ammonia Synthesis Column

Fig. 1 illustrates the information-logical scheme of a three-shelf ammonia synthesis column, where $D_1$and $D_2$denote synthesis gas flow dividers, $P_1$, $P_2$, and $P_3$represent the reactor catalyst shelves, and $TO$denotes the internal heat exchanger.

In the presented scheme, the dashed line outlines the synthesis column itself. The column consists of four main subsystems: three sequentially connected catalyst shelves ($P_1$, $P_2$, $P_3$) and a built-in recuperative heat exchanger ($TO$). In addition, the distribution of synthesis gas flows within the column is controlled by two flow dividers $D_1$and $D_2$.

From the viewpoint of process control, the ammonia synthesis column represents a complex technological object characterized by a large number of disturbance parameters and numerous internal interconnections between process variables.

To address the considered control problem, a mathematical model of the synthesis column has been developed. This model enables the formulation of an optimality criterion for solving the corresponding optimization problem. Although the initial deterministic model obtained at the first stage provides only limited accuracy, it allows the evaluation of the general shape of the objective function over a wide range of argument values, taking into account its possible multiextremal nature and enabling the identification of the region of the global extremum [5, 6].

At the second stage, the model must be identified using experimental data obtained from the real control object. Such data can be collected using probabilistic or experimental identification methods, which allow the influence of various disturbance factors to be taken into account. This approach significantly improves the accuracy of the simulated process parameters.

The development of an adequate mathematical model requires consideration of the nonlinear relationships between the input and output parameters of the technological process. This leads to an increase in the order of the equations describing the control object. However, the use of high-order equations considerably complicates the optimization procedure aimed at determining the optimal process parameters. In many cases, approximate methods have to be applied, which may reduce the accuracy of the developed model [7].

The steady-state operation of the ammonia synthesis column is described by a system of equations presented in [5]. The solution of this system can be expressed as

$$Q_3 = f\left(F_1, F_2, F_3, F_0, F_{цг}, T_{цг}, Q_0, P\right) \quad (1)$$

Equation (1) represents the mathematical model of the three-shelf ammonia synthesis column with respect to the concentration of the target component at the column outlet.

An analysis of the obtained mathematical model indicates that not all variables can be directly determined. Therefore, additional equations must be introduced. To achieve this, the present study proposes the application of test disturbances to the control object. These disturbances involve changing the flow rate of one of the cold bypass streams by a fixed unknown value [4].

For this procedure to be implemented, it is necessary to ensure stabilization of the flow rates in the remaining cold bypass streams during the test conditions. Performing such experiments makes it possible to obtain three additional equations:

$$Q_3' = f_1\left(F_{хб1} + \Delta_1, F_{хб2}, F_{хб3}, (F_0 - \Delta_1), F_{цг}, T_{цг}, Q_0, P\right), \quad (2)$$

$$Q_3'' = f_2\left(F_{хб1}, (F_{хб2} + \Delta_1), F_{хб3}, (F_0 - \Delta_1), F_{цг}, T_{цг}, Q_0, P\right), \quad (3)$$

$$Q_3''' = f_3\left(F_{хб1}, F_{хб2}, (F_{хб3} + \Delta_1), (F_0 - \Delta_1), F_{цг}, T_{цг}, Q_0, P\right). \quad (4)$$

The joint solution of equations (2)–(4) can be written in the following form

$$\begin{aligned} a_4 Q_3^4 + a_3 Q_3^3 + a_2 Q_3^2 + a_1 Q_3 + a_0 = \\ = \phi_1(F_{хб1}) + \phi_2(F_{хб2}) + \phi_3(F_{хб3}) + \phi_{12}(F_{хб1}, F_{хб2}) + \phi_{13}(F_{хб1}, F_{хб3}) + \\ + \phi_{23}(F_{хб2}, F_{хб3}) + \phi_{123}(F_{хб1}, F_{хб2}, F_{хб3}) + \Omega\left(F_{цг}, T_{цг}, Q_0, P\right). \end{aligned} \quad (5)$$

Equation (5) represents a refined mathematical model of the three-shelf ammonia synthesis column equipped with an internal heat exchanger. In this model, the value of the objective function depends on disturbance parameters. Since these parameters can be measured, their values can be substituted directly into equation (5). Moreover, due to the relatively high inertia of the object, disturbance parameters remain nearly constant over relatively long time intervals.

As a result, two values of the target component concentration at the column outlet can be obtained: the measured value and the value calculated by the model. If the calculated value deviates from the measured value beyond a predefined tolerance, the mathematical model must be corrected by recalculating the coefficients $a_4$, $a_3$, $a_2$, $a_1$, and $a_0$.

Solving equation (5) with respect to the concentration of ammonia at the outlet of the synthesis column yields a refined mathematical model describing the column operation. The derivative (or the sum of derivatives) of the concentration with respect to the flow rates of the cold bypass streams equal to zero represents the optimality criterion:

$$\frac{\partial Q}{\partial F_1} + \frac{\partial Q}{\partial F_2} + \frac{\partial Q}{\partial F_3} = 0 \quad (6)$$

Thus, the considered control problem is reduced to the mathematical problem of determining the maximum of a function.

The deterministic modeling approach makes it possible to perform structural identification and determine the general form of the mathematical model of the ammonia synthesis column. In this study, the model is represented by a fourth-order equation with respect to the concentration of the target component. This model forms the basis for the model-based control system of the ammonia synthesis column.

The selected model structure is relatively simple: the unknown variable in the fourth-order equation can be expressed through its coefficients. Therefore, during model adaptation, the functional form of the dependencies remains unchanged, while only the numerical values of the coefficients are updated [4].

During operation of the synthesis column, technological parameters may change under the influence of uncontrolled disturbances that are not included in the model. These disturbances may include variations in the concentration of inert gases in the synthesis gas, catalyst activity degradation, and changes in hydrodynamic regimes inside the column.

Such disturbances may lead to discrepancies between the measured and calculated values of the target component concentration. In this case, it becomes necessary to adjust the coefficients of the left-hand side of the mathematical model ($a_4$, $a_3$, $a_2$, $a_1$, $a_0$). In this work, this problem is solved using the recursive least squares method [6].

After updating the coefficients of the left-hand side of the model, the equality between the left and right sides of the equation is violated. Therefore, the next stage of the adaptation procedure involves adjusting the coefficients of the right-hand side of the model.

Following this procedure, the deterministic model gradually transforms into an experimental-statistical model that reflects the actual operating conditions of the synthesis column.

The obtained mathematical model is subsequently used within the control algorithm to solve the optimization problem.

One of the key process parameters affecting the operation of the synthesis column is the synthesis gas flow rate (unit load). Changes in this parameter lead to a transition of the column to a new steady operating state, which requires additional adaptation of the mathematical model according to the previously described algorithm.

Thus, the proposed approach provides a mechanism for adaptive updating of the mathematical model of the ammonia synthesis column based on a combined deterministic and experimental-statistical modeling framework.

The main task of the control system is to update the model coefficients, solve the optimization problem, and stabilize the flow rates of the cold bypass streams at the calculated optimal values. The solution of the optimization problem involves determining the bypass flow rates that ensure the maximum conversion of synthesis gas into the target product under the current operating conditions.

Due to the complexity of equation (6), the analysis in this work is limited to its general representation. To determine the maximum ammonia concentration at the outlet of the synthesis column for a fixed synthesis gas load $F_{c.g.}$, a multiparameter optimization procedure can be applied. Modern computer-based process control systems make it possible to obtain such solutions within acceptable computational time [8].

However, due to strong uncontrolled disturbances affecting the process, including variations in catalyst activity and hydrodynamic conditions within the column, the solution obtained from the model-based optimization can only be considered as an initial approximation in the vicinity of the optimal operating point.

The operating algorithm of the proposed model-based control system is based on a combined mathematical model of the ammonia synthesis column. A distinctive feature of the proposed modeling approach is that the general structure of the model is obtained using deterministic simulation methods, while the numerical values of the model coefficients are refined through the comparison of simulation results with experimental data obtained from the technological object.

Since the model is represented by a fourth-order equation, the functional dependence of the target component concentration on the process input parameters remains unchanged. This property enables the formulation of an optimization equation that can be used to determine optimal operating conditions. The incorporation of a model adaptation block allows continuous adjustment of the model coefficients and, consequently, of the optimization equation according to the current technological parameters.

Due to the relatively simple mathematical structure of the model and the high computational performance of modern process control systems, the correction of the mathematical model and the optimality criterion equation can be performed in real time. This makes it possible to dynamically determine the optimal values of the key control parameters of the ammonia synthesis process, namely the flow rates of the cold bypass streams supplied to the corresponding catalyst shelves of the synthesis column.

As a result of the conducted research, the technological reserve of the synthesis column in ammonia production has been determined in accordance with the technological regulations. The implementation of the proposed model-based control system makes it possible to stabilize the process at optimal operating conditions and ensure the full utilization of the available technological reserve. Consequently, the application of the developed control system allows increasing the productivity of the ammonia synthesis column by up to 20%.

**Conclusions.** An improved information-logical scheme of the ammonia synthesis column has been developed. The proposed scheme made it possible to determine that the synthesis column is characterized by two input coordinates, three output coordinates, and four disturbance parameters. In addition, the internal interconnections of the control object were clarified and their influence on the output variables of the ammonia synthesis column was analyzed. Based on the obtained results, an operating algorithm for a model-based control system of the ammonia synthesis column was developed.

The general structure of a mathematical model of the ammonia synthesis column with a built-in internal heat exchanger was obtained. This model made it possible to derive a fourth-order optimality criterion equation describing the column operation and to construct the corresponding optimization function.

The proposed approach allows determining the optimal flow rates of the “cold” bypass streams by solving the optimization problem, ensuring that the synthesis column operates under conditions close to the optimal regime. This enables a rapid transition of the control system to the near-optimal operating region. The optimal value of ammonia concentration at the outlet of the synthesis column was determined using the Hooke–Jeeves optimization method, which allows increasing the product yield by up to 1.2 times.

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***Кобзарев Є. В., Дуришев О.А, Куліков Д. О., Лорія М. Г. Розробка алгоритму модельно-орієнтованого керування колоною синтезу аміаку***


*У статті представлено підхід до розроблення модельно-орієнтованої системи керування багатополичною колоною синтезу, що використовується у виробництві аміаку. Запропонований підхід ґрунтується на застосуванні комбінованої математичної моделі, яка поєднує детерміновані та експериментально-статистичні методи моделювання. Таке поєднання дозволяє досягти високого рівня адекватності моделі, забезпечити її адаптивність до змінних умов функціонування та розширити можливості застосування для аналізу й керування складними хіміко-технологічними процесами.*

*На основі запропонованого підходу розроблено математичну модель триполичної колони синтезу аміаку з вбудованим внутрішнім теплообмінником. На основі цієї моделі уточнено інформаційно-логічну схему об'єкта керування, що дало змогу визначити основні внутрішні взаємозв'язки між технологічними параметрами та оцінити їх вплив на вихідні координати колони синтезу. На цій основі розроблено алгоритм функціонування модельно-орієнтованої системи керування.*

*Отриманий математичний опис дозволив сформулювати критерій оптимальності роботи колони та розв'язати задачу оптимізації, спрямовану на визначення оптимальних витрат «холодних» байпасних потоків. Це забезпечує підтримання режиму роботи колони в області, близькій до оптимальної, а також швидкий перехід системи до цієї області під час функціонування. Оптимальне значення концентрації аміаку на виході з колони синтезу визначено із застосуванням методу оптимізації Гука–Дживса.*

*Розроблено функціональну схему автоматизації та проаналізовано комплекс технічних засобів, необхідних для впровадження запропонованої системи керування в промислові автоматизовані системи керування технологічними процесами. Реалізація розробленої модельно-орієнтованої системи керування дозволить зменшити відхилення технологічних параметрів від їх оптимальних значень і підвищити ефективність роботи колони синтезу аміаку.*



***Ключові слова:*** *виробництво аміаку, колона синтезу, модельно-орієнтоване керування, комбінована математична модель, оптимізація процесу.*



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