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CREATION OF AN IDENTIFIER DATABASE FOR THE AMMONIA SYNTHESIS COMPUTER CONTROL SYSTEM

The object of research is the control system of the synthesis department of the large-tonnage ammonia production unit of the AM-1360 series. An analysis of the functioning conditions of the synthesis department was carried out. The significant influence of the content of inerts in the synthesis cycle on the energy efficiency of ammonia production is shown, the optimal value of which depends both on the accepted level of prices for energy carriers and on the method of using purge gases. The need to create a computer-integrated control technology to optimize the use of purge gases is established. The function of the identifier of such a control technology is defined, namely, continuous refinement based on current information about the state of the main sections of the synthesis department, such as the synthesis column, primary and secondary condensation. The operation of these stations takes place in the conditions of seasonal and daily changes in the heat load, which causes parametric uncertainty of such parameters of the connection of the mathematical model as the concentration of ammonia in the circulating gas at the outlet of the stations listed above. Numerical assessment of these uncertainties according to the results of analytical studies for such technological objects is most often performed using stochastic approximation methods. Let's note that the significant inertia of the objects of the synthesis department under certain conditions makes it impossible to adapt the parameter to its actual value.

An algorithmic base has been created for the formation of an information array of the identifier of the computer-integrated control technology of the ammonia synthesis department, which ensures the separation of transient modes under conditions of uncertainty and allows to perform the task of identifying processes in the synthesis column, in the primary and secondary condensation units. The proposed algorithm allows to perform convergence in the department both on the general and on the component material balances. The algorithm is implemented in the MatLab application program package and tested by means of simulation based on experimental data of industrial operation of AM-1360 series ammonia synthesis units.

Keywords: *algorithmic database, identifier, computer-integrated control system, ammonia production.*

1. Introduction

Modern large-tonnage production of ammonia is a multi-stage energy technological complex. One of the most important final stages of such productions is the division of ammonia synthesis. The synthesis department, where production ammonia is actually obtained, is based on the traditionally accepted closed Haber-Bosch circulation scheme [1] with a two-stage condensation system, which is carried out by cooling the circulating gas (CG). The widespread use of air and water cooling devices in ammonia condensation systems due to changes in the parameters of the external environment causes parametric uncertainty in the functioning of the synthesis department. Under such conditions, as a result of temperature fluctuations of primary and secondary condensation in the ranges from 26 °C to 36 °C and from –8 °C to +5 °C, respectively, a significant change in the

composition of CG occurs both at these stations and at the outlet of the synthesis column. At the same time, the content of inerts in CG varies within a fairly wide range from 12 % by volume to 15 % by volume [2]. However, as noted in [3], the content of inerts significantly affects the energy efficiency of ammonia production, the optimal value of which depends on both the accepted level of energy prices and the method of using purge gases. Thus, a certain scheme of the ammonia synthesis unit determines the need to determine the optimal flow of purge gases, and therefore the concentration of inerts in the synthesis cycle. Therefore, optimization of the process of removing purge gases in the synthesis cycle due to the creation of computer integrated control technologies is an urgent problem in increasing the energy efficiency of ammonia production.

According to literary sources [4–6], the creation of such a computer-integrated control technology under conditions

of uncertainty requires the use of an adaptive system, the main elements of which are an identifier with a mathematical model. The identifier provides continuous refinement of the model based on current information about the state of the synthesis department, in particular, its main sections – the synthesis column, primary and secondary condensation. The operation of these stations takes place in the conditions of seasonal and daily changes in heat load, which causes parametric uncertainty of the main parameters of the connection of the mathematical model. Among these parameters, those that determine the efficiency of the processes should be noted, namely, the concentration of ammonia in the circulation gas at the outlet of the above-mentioned stations [7]. Numerical evaluation of these uncertainties for such linear technological objects is most often performed using the stochastic approximation method [8, 9]. However, this process is complicated by the significant inertia of objects in selected sections of the synthesis department, such as, for example, a condensation column (over 10 tons) or a synthesis column (over 484 tons without a catalyst). All this, under certain conditions, makes it impossible to adapt the parameter to its actual value. Therefore, *the aim of the study* is to create an algorithmic basis for the formation of an information array for the separation of transient modes of the synthesis department. What is necessary under such circumstances is to perform the identification of non-stationary technological objects, in particular, the synthesis column, the primary and secondary condensation sites for the purpose of numerical assessment of ammonia concentrations at the outlet of the listed sites.

2. Materials and Methods

The research was carried out based on the data obtained on the AM-1360 series industrial synthesis unit. The collection of experimental data on the real parameters of the operation of the synthesis department of the industrial unit was carried out using the means of the TDC-3000 microprocessor information and control complex of the company «Honeywell» and partially laboratory analyses. The generalized block diagram of the ammonia synthesis department with the main parameters control points according to the technological regulation is shown in Fig. 1.
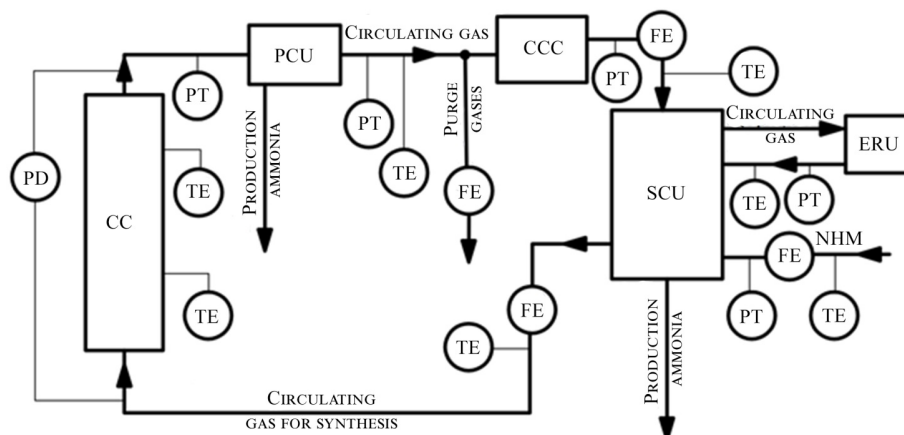
Sampling for laboratory analyzes to determine the composition of gas (ammonia, argon, methane, nitrogen, hydrogen) at the inlet and outlet of the condensation column of the secondary condensation unit was carried out once per shift. At the same time, an additional analysis of CG for ammonia content was performed directly after the synthesis column. In this regard, the frequency of collection of all other data on the work parameters of the synthesis department also occurred once per shift. The content of ammonia in CG was determined in laboratory conditions, and the composition of other components of CG was carried out by the workshop laboratory using an industrial chromatograph NeoCHROM (Ukraine).

3. Results and Discussion

In the process of creating an algorithmic base for the formation of the information array of the identifier, the equations of the mathematical description of the material balance of the ammonia synthesis department were used [7]. The algorithm contains two cycles of material balance convergence. Does the former make a difference? Which ensure the convergence of material flows at the stage of primary condensation. The second cycle ensures the convergence of material flows at the stage of secondary condensation, which ensures consistency not only in terms of the general, but also in terms of the component material balance of the synthesis department as a whole.

At the same time, the algorithm includes the following functional blocks:

Block 1. Calling the problem to a solution after a certain time interval or at the command of the operator.

Block 2. Opening the BASA file that serves this task.

Block 3. Subroutine for reading the necessary information from the DANI file, which stores information about input and output variables received from the TDC-3000 information and control complex.

Block 4. Determination of the productivity G_C of the ammonia synthesis column according to the equation:

$$G_C = \frac{V_C^{IN}\left(Y_C^{OUT} - Y_C^{IN}\right)}{100 + 1.0316 Y_C^{OUT}}, \tag{1}$$

where V_C^{IN} – CG consumption at the input of the synthesis column, nm^3/s; Y_C^{IN}, Y_C^{OUT} – ammonia concentration in CG, respectively at the input and output of the synthesis column according to industrial operation data, % vol.

Block 5. Performing calculations of CG consumption V_C^{OUT}, concentration of inerts in CG at the output of the synthesis column according to the formulas:

$$V_C^{OUT} = V_C^{IN} - G_C; \tag{2}$$

$$I_C^{OUT} = \frac{V_C^{OUT} I_C^{IN}}{V_C^{OUT}}, \tag{3}$$

where I_C^{IN} – concentration of inerts in the CG at the input of the synthesis column according to industrial operation data, vol. dollars.

Block 6. Determination of the solubility of nitrogen-hydrogen

Fig. 1. Generalized block diagram of the ammonia synthesis department with the main parameters control points using the TDC-3000 information and control complex: CC – synthesis column; PCU – primary condensation unit; CCC – circulation compressor; SCU – secondary condensation unit; ERU – evaporators of refrigerating units; NHM – nitrogen-hydrogen mixture; PD – pressure drop sensor; PT – pressure sensor; TE – temperature sensor; FE – flow sensor

mixture (NHM), argon and methane in liquid ammonia at the temperature of primary and secondary condensation according to formulas approximating experimental data [10]:

$$\upsilon_{CH_4}^P = (0.185 + 0.0036t)10^{-3};$$ (4)

$$\upsilon_{Ar}^P = (0.085 + 0.0014t)10^{-3};$$ (5)

$$\upsilon_{NHM}^P = 0.7 \cdot 10^{-4} + 0.242 \cdot 10^{-4}\left(\frac{t-20}{20}\right) +$$
$$+ 0.23 \cdot 10^{-5}\left(\frac{t-20}{20}\right)^2,$$ (6)

where t – temperature according to industrial operation data, °C; υ – solubility of gases, m³/(kgf/cm²).

Block 7. Calculation of the specific amount of dissolved gases (m³/m³ of liquid ammonia) in primary and secondary condensation units according to the equation [10]:

$$\upsilon^P = \frac{10.2P^{OUT}}{100}\left(\upsilon_{CH_4}^P a_{CH_4}^{OUT} + \upsilon_{Ar}^P a_{Ar}^{OUT} + \upsilon_{NHM}^P a_{NHM}^{OUT}\right),$$ (7)

where P^{OUT} – condensation pressure at the outlet of the corresponding condensation units, MPa; $a_{CH_4}^{OUT}, a_{Ar}^{OUT}, a_{NHM}^{OUT}$ – respectively, the concentration of ammonia, argon and nitrogen-water mixture at the output of the corresponding condensation units according to industrial operation data, % vol.

Block 8. The yield of condensed ammonia from the unit of primary G_{PC} and secondary G_{SC} condensation is determined by the formulas:

$$G_{PC} = \frac{V_C^{IN}\left(Y_{PC}^{IN} - Y_{PC}^{OUT}\right)}{100 - Y_{PC}^{OUT}\left(1 + \upsilon_{PC}^P\right)};$$ (8)

$$G_{SC} = G_C - G_{PC} - V_P Y_{PC}^{OUT}/100,$$ (9)

where $Y_{PC}^{IN}, Y_{PC}^{OUT}$ – concentration of ammonia in CG, respectively, before and after primary condensation, % vol.; V_P – consumption of purge gases according to industrial operation data, nm³/s.

Block 9. Determination of gas consumption V^P dissolved in liquid ammonia in condensation units according to the following equations:

$$V_{CH_4}^P = 10\upsilon_{CH_4}^P P^{OUT} G \cdot a_{CH_4}^P/100;$$ (10)

$$V_{Ar}^P = 10\upsilon_{Ar}^P P^{OUT} G \cdot a_{Ar}^P/100;$$ (11)

$$V_{ABC}^P = 10\upsilon_{ABC}^P P^{OUT} G \cdot a_{NHM}^P/100;$$ (12)

$$V^P = V_{CH_4}^P + V_{Ar}^P + V_{ABC}^P;$$ (13)

$$V_i^P = V_{CH_4}^P + V_{Ar}^P,$$ (14)

where V_i^P – consumption of inerts dissolved in liquid ammonia in condensation units, nm³/s; G – output of condensed ammonia for the corresponding condensation unit (G_{PC} or G_{SC}), nm³/s.

Block 10. Calculation of CG consumption at the input of the secondary condensation unit V_{SC}^{IN}, CG consumption V_{PC}^{OUT}, concentration of inerts in CG at the output of the primary condensation unit according to the formulas:

$$V_{PC}^{OUT} = V_C^{OUT} - G_{PC} - V_{PC}^P;$$ (15)

$$I_{PC}^{OUT} = \frac{V_C^{OUT} I_C^{OUT} - V_{iPC}^P}{V_{PC}^{OUT}};$$ (16)

$$V_{SC}^{IN} = V_{SC}^{OUT} - V_P,$$ (17)

where I_S^{OUT} – concentration of inerts in the CG at the outlet of the synthesis column, vol. %; V_{iPC}^P – consumption of dissolved inerts in liquid ammonia of the primary condensation unit, nm³/s.

Block 11. Evaluation of the error of convergence δ_1 and δ_2 with respect to the balance at the stage of primary condensation according to the equations:

$$\delta_1 = \frac{I_{PC}^{OUT} - I_{PC.E}^{OUT}}{I_{PC}^{OUT}}100 \leq 3~\%;$$ (18)

$$\delta_2 = \frac{V_{PC}^{IN} - V_{PC.E}^{IN}}{PC}100 \leq 3~\%,$$ (19)

where $I_{PC.E}^{OUT}$ – concentration of inerts in the CG at the inlet of the primary condensation unit according to industrial operation data, vol. %; $V_{PC.E}^{OUT}$ – CG consumption at the input of the secondary condensation unit according to industrial operation data, nm³/s.

If the conditions (18) and (19) are fulfilled, the transition to the calculation of the consumption of condensed ammonia at the stage of secondary condensation is carried out.

Block 12. Determination of the amount of ammonia G_E that evaporates in the condensation column due to the increase in the temperature of liquid ammonia due to the introduction of fresh NHM according to the equation:

$$G_E = V_0 \frac{Y_C^{OUT}}{100 - V_i^{IN}},$$ (20)

where V_0 – consumption of fresh NHM to the condensation column according to industrial operation data, nm³/s.

Block 13. The amount of condensed liquid ammonia G_{EA} in the condensation column without taking into account the process of its evaporation is calculated by the formula:

$$G_{EA0} = \frac{V_{SC}^{IN}\left(Y_{PC}^{OUT} - Y_C^{IN}\right)}{100 - Y_i^{IN}\left(1 + \upsilon_{EA}^P\right)}.$$ (21)

Block 14. The amount of liquid ammonia remaining in the condensation column after evaporation is determined by the equation:

$$G_{EA} = G_{EA0} - \Delta G_E.$$ (22)

Block 15. Evaluation of the balance convergence error δ_3 regarding the stage of secondary condensation according to the equation:

$$\delta_3 = \frac{G_{EA} - G_{EA.E}}{G_{EA}}100 \leq 3~\%.$$ (23)

Block 16. Formation of an array of current STAB data of stable values regarding the material flows of the concentration of components in the central heating system, pressure and temperature at the stations of primary and secondary condensation and ammonia synthesis column and printing of the results.

Block 17. Closing the STAB file and exiting the task.

The developed structure of the algorithm makes it possible to form a stable (static) information array of current data and to separate transient modes. This will make it possible to carry out a numerical assessment of uncertainties using the method of stochastic approximation based on the obtained array of experimental data. The algorithm is implemented in the MatLab package and tested on the data of the industrial operation of the ammonia synthesis unit of the AM-1360 unit.

4. Conclusions

Based on the research results, an algorithmic base was created for the formation of an information array of the identifier of the computer control system of the department of synthesis of ammonia production, which ensures the separation of transient dynamic modes under conditions of uncertainty. This allows further numerical assessment of the uncertainties of the main parameters of the relationship of the mathematical model of the synthesis unit, namely the concentration of ammonia in the CG at the outlet of the synthesis column, primary and secondary condensation units. In this way, identification of the processes of stationary static technological objects of the department of synthesis of ammonia production is ensured.

The algorithm for forming the information array was implemented in the MatLab package and tested by means of simulation modeling based on experimental data of industrial operation of AM-1360 series ammonia synthesis units operating in Ukraine.

The research results can be used to determine the optimal consumption of purge gases in the cycle of ammonia synthesis, as well as the optimal temperature of primary condensation.

The presented algorithm is limited to the technological design of condensation systems used in the synthesis department.

Further research will be aimed at using the developed algorithm in intelligent control systems in order to increase the energy efficiency of ammonia production.

Conflict of interest

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

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Data availability

Manuscript has no associated data.

Use of artificial intelligence

The authors confirm they did not use artificial intelligence technologies when creating the presented work.

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