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## **ASSESSMENT OF THE FORECAST OF THE OPERATING MODE OF THE COMPLEX OF AMMONIA SECONDARY CONDENSATION PRODUCTION IN UNCERTAINTY CONDITIONS**

**Abstract.** The article describes the analysis of conditions of secondary condensation complex functioning. There, the software algorithm for estimating the forecasts of functioning mode is developed, which makes it possible to prepare the complex operator in conditions of existing uncertainty for making decisions in supervisor control mode.

**Keywords:** secondary condensation, ammonia production, forecast evaluation, uncertainty conditions.

One of the most crucial stages of separation of ammonia synthesis of AM-1360 series units operating in Ukraine is secondary condensation, which performs the final removal of commercial ammonia from the synthesis cycle. Previous studies have improved the energy efficiency of the secondary condensation stage by creating an optimal structure that ensures the exclusion of electrically driven turbo-compressor refrigeration unit from the operational scheme and reducing the thermal load on low-temperature evaporators (LTE) [1; 2]. Technological

complex of this structure is formed by additional heat exchanger (AH), condensing column (CC), high-temperature evaporator (HTE) with steam-jet refrigerating unit (SJRU) and two LTEs with water-ammonia refrigerating units (WACU).

Functioning of the secondary condensation complex is done under conditions of uncertainty [3], which is mainly due to constant changes in the external heat load due to the application of air-cooled circulating gas (CG) units at the previous stage of primary condensation and the lack of pos-

sibility of continuous automatic control of ammonia concentration in CG [4]. At the same time, the range of changes at the inlet of the complex temperature of the CG and ammonia concentration in the CG is  $35 \div 45$  °C and  $8.6 \div 12\%$  respectively. Under such circumstances, the CG temperature at the HTE inlet, which is included in the SJRU operational scheme, will also change. Therefore, it is necessary to apply a control system to stabilize the CG temperature at the CC inlet at 30 °C, and therefore stabilize the CG temperature at the HTE inlet at 9.2 °C, which was provided by the functional scheme of secondary condensation process control [5].

However, the process equipment of the complex of secondary condensation is characterized by significant inertia, which is due to its large metal intensity. Only the mass of CC is about 290 tons [6]. At the same time, SJRU is a rather complicated technological system in which change of refrigerating capacity and, consequently, expenses of the coolant to HTE are in general performed at the expense of changing the number of working ejectors [7]. Therefore, for the purpose of increasing control reliability and possibility of preparation of the operator for such changes in the supervisor control mode, which is provided by the functional control scheme, a subsystem of decision making support is necessary. It should provide assessment of forecasts of possible changes in CG temperature at the inlet of HTE. Setting of this temperature will condition the determination of forecast of necessary SJRU refrigerating capacity and, consequently, of coolant costs to HTE and monoethanolamine (MEA) solution to SJRU steam generator, which provides necessary supply of working steam/vapor for ejection of the coolant from HTE.

In the process of algorithm development there have been used equations of mathematical description of AH heat exchange, HTE evaporator, subroutine of calculation of heat transfer coefficients, heat transfer and ammonia concentration in AH at the inlet and outlet of secondary condensation complex  $a_{NH_3}^{IN}$  and  $a_{NH_3}^P$  according to the developed algorithms

stated in [4; 8] and located in STAB and STOCH files. The algorithm contains convergence cycles, which provide alignment of heat flows from the side of the pipe and inter-pipe space and in the process of heat exchange AH to determine the temperature of CG at the outlet of its inter-pipe space. Then according to this temperature the necessary cooling capacity of SJRUs is sequentially determined, which will condition the stabilization of AH temperature at the outlet of HTEs at the level of 30 °C, coolant consumption in HTEs for its provision, consumption of working ammonia vapor for ejection and consumption of IEA solution for obtaining this vapor in SJRUs steam generator. At that the algorithm contains the following main functional blocks.

*Block 1.* Call of the task to be solved in a certain period of time or by operator's command.

*Block 2.* Open the PROG file that serves this task.

*Block 3.* A sub-program for reading the necessary DANI file information, which receives and stores the current information about inlet and outlet variables and structural characteristics of the object, obtained from the information management complex TDC-3000.

*Block 4.* STAB data reading sub-program for determining heat transfer coefficients of actual  $K_E^A$  and calculated according to formulas accepted at design  $K_D^A$ .

*Block 5.* STOCH sub-program on fulfillment of stationary conditions, process reproducibility and hypothesis on normality of empirical distribution and determination of functional dependencies for numerical estimation of volume concentrations of ammonia in CG at inlet  $a_{NH_3}^{IN}$  and outlet  $a_{NH_3}^P$  of secondary condensation complex using MATLAB (Optimization Toolbox) package, which according to research [4] should be calculated using equations:

$$a_{NH_3}^{IN} = f(P_{PC}, \Theta_{PC}); \quad (1)$$

$$a_{NH_3}^{TP} = f(V_{NHM}, V_{IP}^{CG}, \Theta_P^{LTE}, a_{NH_3}^{IN}, P_{CG}), \quad (2)$$

where  $P_{PC}$ ,  $P_{CG}$  are primary condensation pressure and CG at the AH inlet, MPa;  $\Theta_{PC}$ ,  $\Theta_P^{LTE}$  are primary

condensation temperature and CG respectively at the outlet of *LTE*, °C;  $V_{NHM}$ ,  $V_{IP}^{CG}$  are volume flow rate of nitrogen-hydrogen mixture (NHM) and CG at the inlet of AH, nm<sup>3</sup>/s.

*Block 6.* Determination of condensed ammonia flow rate  $M_{CD}^{AH}$  in CG flow of inter-pipe space AH and total thermal resistance  $R_T^{EA}$  is done using the following equations:

$$M_{CD}^{AH} = 0.771 V_{IP}^{CG} (a_{NH_3}^{IN(v)} - a_{NH_3}^{OUT(v)}); \quad (3)$$

$$a_{NH_3}^{IN(v)} = \frac{P_{NH_3}^{IN}}{P_{CG}}; \quad (4)$$

$$a_{NH_3}^{OUT(v)} = \frac{P_{NH_3}^{OUT}}{P_{CG}}; \quad (5)$$

$$R_T^{EA} = \frac{1}{K_E^A} - \left( \frac{1}{\alpha_p^A} + \frac{1}{\alpha_{IP}^A} \right), \quad (6)$$

where  $a_{NH_3}^{IN(v)}$ ,  $a_{NH_3}^{OUT(v)}$  are, respectively, the concentration of ammonia vapour in the CG inlet and outlet of AH, volume ratio;  $P_{NH_3}^{IN}$ ,  $P_{NH_3}^{OUT}$  is the partial pressure of ammonia vapor in CG correspondingly at inlet and outlet of inter-pipe space of AH, MPa;  $\alpha_p^A$ ,  $\alpha_{IP}^A$  – are the coefficients of heat transfer correspondingly from the side of pipe and inter-pipe space, calculated by Krausold equations, W/(m<sup>2</sup> · K) [1].

*Block 7.* Subprogram of calculating the functional dependence on the numerical estimate of uncertainty  $R_T^{EA}$  using the MATLAB (Optimization Toolbox) software, which should be searched by equation [1]:

$$R_T^{EA} = f(M_{CD}^{AH}) \quad (7)$$

*Block 8.* Flow rate of CG  $M_p^A$  (kg/s) at CC outlet is determined by the following formulas:

$$M_{CD}^{CC} = \frac{V_{IP}^A (a_{NH_3}^{IN} - a_{NH_3}^P) 0.771}{100 - a_{NH_3}^P}; \quad (8)$$

$$G_{EV}^S = V_{NHM} \frac{a_{NH_3}^P 0.771}{100 - a_{NH_3}^P}; \quad (9)$$

$$M_V^{CC} = M_{CD}^{CC} - G_{EV}^S; \quad (10)$$

$$M_p^A = M_{IP}^A - M_V^{CC}, \quad (11)$$

where  $M_{CD}^{CC}$ ,  $G_{EV}^S$ ,  $M_V^{CC}$  is the flow rate of ammonia, respectively, condensed into CC, obtained by evaporation during the heat exchange with NHM and liquid ammonia from CC, kg/s;  $V_{IP}^A$ ,  $V_{NHM}$  are, re-

spectively, the volume flow rate of CG at the AH inlet and nitrogen-hydrogen mixture at the CC inlet, nm<sup>3</sup>/s.

*Block 9.* Setting the initial temperature approximation  $\Theta_p^{CG} = \Theta_p^{CC} + \Delta\Theta$  at the outlet of the AE pipe space with determination of the heat flow  $\Phi_p^A$  from the AE pipe space by the following formula:  $\Phi_p^A = M_p^{AG} C_p^{AG} (\Theta_p^{CG} - \Theta_p^{CC}) + M_L^{AIN} (i_L^{AIN} - i_V^{AOUT})$ , (12) where  $M_p^{AG}$ ,  $M_L^{AIN}$  are respectively the mass flow rate of CG gas mixture at the outlet and liquid ammonia at the outlet of the AE pipe space, kg/s;  $C_{TP}^{AG}$  is the average heat capacity of CG gas mixture, kJ/(kg·K);  $i_L^{AIN}$ ,  $i_V^{AOUT}$  are respectively the enthalpy of liquid ammonia at the outlet and ammonia vapor at the outlet of the AE pipe space, kJ/kg;  $\Theta_p^{CC} = 17.5$  °C is the CG temperature at inlet of AE pipe space, which is provided by CG temperature at CC inlet at the following level  $\Theta_{2CG}^{HTE} = 30$  °C and CG temperature at *LTE* outlet at the following level  $\Theta_p^{LTE} = -5$  °C;  $\Delta\Theta$  – approximation step, °C.

*Block 10.* Setting the initial temperature approximation  $\Theta_{1CG}^{HTE} = \Theta_{IP}^{CG} - \Delta\Theta$  at the outlet of the AE inter-pipe space with determination of the amount of condensed ammonia  $M_{CD}^A$  according to equations (3–5) and heat flow  $\Phi_{IP}^A$  from the AE inter-pipe space according to the following formula:

$$\Phi_{IP}^A = M_{IP}^{AG} C_{IP}^{ACG} (\Theta_{IE}^{CG} - \Theta_{1CG}^{HTE}) + M_{CD}^A r_{IN}^A + (M_L^A - 0.5 M_{CD}^A) C_L^A (\Theta_{IP}^{CG} - \Theta_{1CG}^{HTE}) \quad (13)$$

where  $M_{IP}^{AG}$ ,  $M_{CD}^A$ ,  $M_L^A$  – are respectively the amount of gas mixture at the outlet of the AE inter-pipe space, condensed and liquid ammonia space in the AE inter-pipe space, kg/s;  $C_{IP}^{ACG}$ ,  $C_L^A$  are respectively the average heat capacity of gas mixture of AE inter-pipe space and liquid ammonia, kJ/(kg·K);  $r_{IN}^A$  is specific heat of condensation in the AE inter-pipe space, kJ/kg;  $\Theta_{IP}^{CG}$  is the temperature of CG at the inlet of the AE inter-pipe space, °C.

*Block 11.* Estimation of error margin of convergence condition  $\delta_1^A$  of heat flows  $\Phi_p^A$  and  $\Phi_{IP}^A$  and transition in case of its fulfillment to calculation of heat flow  $\Phi_T^A$  due to heat exchange according to the following formulas:

$$\Phi_T^A = K_E^A F_A \Delta\Theta_{MN}^A; \quad (14)$$

$$K_E^A = \frac{1}{\frac{1}{\alpha_p^A} + \frac{1}{\alpha_{IP}^A} + R_T^{EA}}, \quad (15)$$

where  $F_A = 1150$  is the surface of heat exchange of AE, m<sup>2</sup>;  $\Delta\Theta_{MN}^A$  is the log mean temperature difference of AE, °C.

$$M_{IN}^{HTE} = \frac{M_P^{HTE} C_P^{CG} (\Theta_{1CG}^{HTE} - \Theta_{2CG}^{HTE}) + M_{CD}^{HTE} r_{CD} + (M_L^{HTE} - 0.5 M_{CD}^{HTE}) C_L^{HTE} (\Theta_{1CG}^{HTE} - \Theta_{2CG}^{HTE})}{r_{CL} - (\Theta_{CL1} - \Theta_{CL2})}, \quad (16)$$

where  $M_P^{HTE}$ ,  $M_{CD}^{HTE}$ ,  $M_L^{HTE}$  is the flow rate of gas mixture, condensed ammonia and liquid ammonia respectively in the pipe space of the HTE, kg/s;  $C_P^{CG}$ ,  $C_L^{HTE}$  are the average heat capacity of gas mixture and liquid ammonia respectively in the pipe space of the HTE, kJ/(kg·K);  $r_{CD}$ ,  $r_{CL}$  is heat of ammonia condensation and vaporization in pipe and inter-pipe space of HTE, kJ/kg;  $\Theta_{CL1}$  is coolant (ammonia) temperature at HTE inlet, °C;  $\Theta_{CL2} = 24$  is the coolant boiling point in inter-pipe space of HTE, °C.

*Block 13.* Calculation of the flow rate of working ammonia vapor  $M_V$  to SJRU ejectors, MEA solution flow  $M_{MEA}$  to produce this vapor, as well as the total amount of coolant vapor and  $M_{TTL}$  working vapor to air condensers according to the following formulas:

$$M_{MEA} = \frac{M_V r_V}{C_{MEA} (\Theta_{MEA1} - \Theta_{MEA2})}; \quad (17)$$

*Block 12.* Estimation of error margin of convergence condition  $\delta_2^A$  of heat flows  $\Phi_p^A$ ,  $\Phi_{IP}^A$  and  $\Phi_T^A$  and in case of its fulfillment, given determined temperature  $\Theta_{1CG}^{HTE}$  transition to the calculation of  $M_{IN}^{HTE}$  (kg/s) at the inlet of HTE inter-pipe space according to the equation:

$$M_V = \frac{M_{IN}^{HTE}}{u}; \quad (18)$$

$$M_{TTL} = M_V + M_{MEA}, \quad (19)$$

where  $r_V$  is the specific heat of ammonia vaporization at 65 °C and pressure of 3 MPa, kJ/kg;  $C_{MEA}$  is the specific heat capacity of MEA solution, kJ/(kg·K);  $\Theta_{MEA1} = 85$  °C,  $\Theta_{MEA2} = 75$  °C is the temperature of MEA solution at inlet and outlet respectively;  $u = 0.4$  – ejection coefficient [7].

*Block 14.* Formation of PSPR current data array of the decision-making subsystem, in particular  $M_V$ ,  $M_{MEA}$ ,  $M_{TTL}$  and formation of results.

*Block 15.* Closing the PROG file and task termination.

Table 1 shows, as an example, separate results of calculations according to the given algorithm, implemented in the MATLAB R2014a software.

Table 1.– Separate results of assessment of forecasts of the subsystem of support for management decision making in the conditions of changes in CG temperature at the secondary condensation complex inlet with ammonia concentration in CG at the inlet of 10.1% vol

Performance data	CG temperature at the secondary condensation complex inlet $\Theta_{IP}^{CG}$ , °C		
	37	41	45
<b>I</b>	<b>2</b>	<b>3</b>	<b>4</b>
Additional heat exchanger (AH)			
Heat flow $\Phi_T^A$ , MW	3.31	4.25	5.19
Heat transfer coefficient $K_E^A$ , W/(m <sup>2</sup> ·K)	304.86	343.83	376.04
Temperature at the outlet of the inter-pipe space $\Theta_{1CG}^{HTE}$ , °C	30.40	32.76	35.17
Temperature at the outlet of the pipe space $\Theta_p^{CG}$ , °C	30.32	33.79	37.31

<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>
Amount of condensed ammonia in the inter-pipe space $M_{CD}^A$ , t/h	5.33	7.15	9.14
Log mean temperature difference $\Delta\Theta_{MN}^A$ , °C	9.45	10.74	11.99
High Temperature Evaporator and SJRU			
Heat flow $\Phi_{HTE}$ , MW	0.19	1.36	2.57
Amount of condensed ammonia in the pipe space $M_{CD}^{HTE}$ , t/h	0.30	2.11	4.07
Coolant quantity at the inlet of the inter-pipe space $M_{IN}^{HTE}$ , t/h	0.64	4.44	8.38
Quantity of working ammonia vapor to SJRU ejectors $M_V$ , t/h	1.59	11.09	20.96
MEA solution quantity for working vapor $M_{MEA}$ , t/h	41.06	285.84	540.29

The developed algorithmically-programmed software of the decision support subsystem allows to predict the modes of its functioning for such a complex inertial object with high metal intensity as a complex of secondary condensation. It gives

an opportunity to prepare the complex operator in conditions of existing uncertainty for decision-making in the supervisor control mode in order to stabilize the temperature conditions of circulating gas cooling.

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