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Modeling the dynamic mode of the chlorinator in the production of chloromethane

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In the production of chloromethane the main apparatus is a chlorinator, which in the production of chloromethane is used directly for chlorination of methane, this procedure requires a clear temperature regime, heating occurs by supplying heating gases from the furnace where the process of burning natural gas in excess air.

The main initial parameter (adjustable value) is the temperature of the reaction gases at the outlet of the chlorinator $\theta out_{\text{р.г}}$.

Inlet (control signal, control action) - air flow at the inlet to the furnace $G_{\text{пов}}$. The perturbation is the consumption of reaction gases at the entrance to the apparatus $\theta in_{\text{р.г}}$.

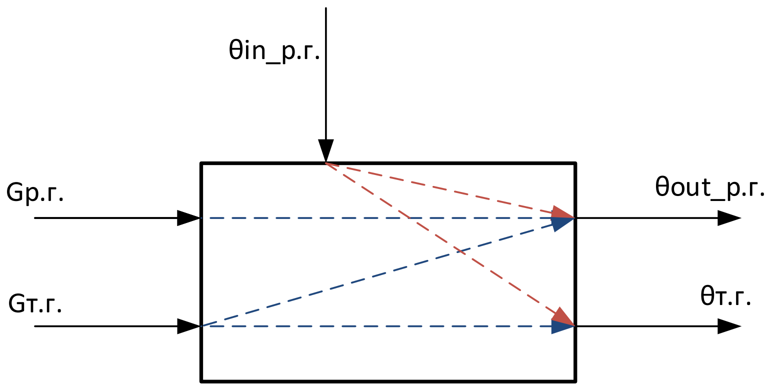

Fig. 1. Structural and parametric scheme of the chlorinator.

$G_{\text{р.г}}$ – consumption of reaction gases; $\theta in_{\text{р.г}}$ – temperature of reaction gases at the inlet; $\theta out_{\text{р.г}}$ - temperature of reaction gases at the outlet; $G_{\text{т.г}}$ – flue gas consumption; $\theta_{\text{т.г}}$– temperature of flue gases;

According to the technology of methane chlorination, it is necessary that the temperature of the reaction gases was 450 °C. Temperature control will be carried out through the channel «air flow - outlet temperature of reaction gases».

Equation of heat balances:

$$\begin{cases} G_{\text{р.г}} \cdot c_{\text{р.г}} \cdot \theta in_{\text{р.г}} + G_{\text{т.г}} \cdot c_{\text{т.г}} \cdot \theta_{\text{т.г}} + q_r \cdot k \cdot {x_b}^m = G_{\text{р.г}} \cdot c_{\text{р.г}} \cdot \theta out_{\text{р.г}} \\ G_{\text{п}} \cdot c_{\text{п}} \cdot \theta_{\text{п}} + \alpha \cdot G_{\text{пов}} \cdot c_{\text{пов}} \cdot \theta_{\text{пов}} = G_{\text{т.г}} \cdot c_{\text{т.г}} \cdot \theta_{\text{т.г}} \end{cases} \quad (1)$$

Table 1 Values of the main static mode

Name	Marking	Numeric value	Dimensionality
Consumption of reaction gases	$G_{р.г}$	0,5	kg / s
Flue gas consumption	$G_{т.г}$	0,02	kg / s
Fuel consumption	$G_п$	0,02	kg / s
Density of flue gases	$\rho_{т.г}$	1,22	kg / m^3
Density of reaction gases	$\rho_{р.г}$	1,4	kg / m^3
Reaction gas temperature (inlet)	$\theta in_{р.г}$	100	˚C
Heat capacity of reaction gases	$c_{р.г}$	1.430	kJ / (kg · K)
Heat capacity of fuel	$c_п$	2.226	kJ / (kg · K)
Heat capacity of air	$c_{пов}$	1.007	kJ / (kg · K)
Heat capacity of flue gases	$c_{т.г}$	20.07	kJ / (kg · K)
Energy of activation of a chemical reaction	$E_а$	83.7	kJ
Energy is attributed to 1 mole of substance	q_r	62.31	kJ
Volume of reaction gases	$V_{р.г}$	1.5	m^3
Volume of flue gases	$V_{т.г}$	2.5	m^3

From the equation of the second equation of the system (1) we derive the equation of dynamics, where the input parameter is $G_{пов}$, and the output – $\theta_{т.г}$:

$$G_п \cdot c_п \cdot \theta_п + \alpha \cdot G_{пов} \cdot c_{пов} \cdot \theta_{пов} - G_{т.г} \cdot c_{т.г} \cdot \theta_{т.г} = V_{т.г} \cdot c_{т.г} \cdot \rho_{т.г} \frac{d\theta_{т.г}}{dt} \quad (2)$$

$$\Delta G_п \cdot c_п \cdot \theta_п + \alpha \cdot \Delta G_{пов} \cdot c_{пов} \cdot \theta_{пов} - G_{т.г} \cdot c_{т.г} \cdot \Delta\theta_{т.г} = V_{т.г} \cdot c_{т.г} \cdot \rho_{т.г} \frac{d\Delta\theta_{т.г}}{dt} \quad (3)$$

$$\Delta G_п \cdot \frac{c_п \cdot \theta_п}{G_{т.г} \cdot c_{т.г}} + \Delta G_{пов} \cdot \frac{\alpha \cdot c_{пов} \cdot \theta_{пов}}{G_{т.г} \cdot c_{т.г}} = \frac{V_{т.г} \cdot c_{т.г} \cdot \rho_{т.г}}{G_{т.г} \cdot c_{т.г}} \cdot \frac{d\Delta\theta_{т.г}}{dt} + \Delta\theta_{т.г} \quad (4)$$

$$T1 = \frac{V_{т.г} \cdot c_{т.г} \cdot \rho_{т.г}}{G_{т.г} \cdot c_{т.г}} \qquad k_{Gt\_\theta tg} = \frac{c_п \cdot \theta_п}{G_{т.г} \cdot c_{т.г}} \qquad k_{Gair\_\theta tg} = \frac{\alpha \cdot c_{пов} \cdot \theta_{пов}}{G_{т.г} \cdot c_{т.г}} \quad (5)$$

Equations in canonical form

$$k_{Gt\_\theta tg}\Delta G_{п} + k_{Gair\_\theta tg}\Delta G_{пов} = T1\frac{d\Delta\theta_{т.г}}{dt} + \Delta\theta_{т.г} \quad (6)$$

Perform the transformation of equation (6) according to Laplace

$$\theta_{т.г} = \frac{k_{Gair\_\theta tg}\Delta G_{пов}}{T1 \cdot p + 1} \quad (7)$$

Substituting in the first equation of the system (1) equation (7) we derive the equation of dynamics, where the input parameter is

$G_{пов}$, and the output – $\theta out_{р.г}$:

$$G_{р.г} \cdot c_{р.г} \cdot \theta in_{р.г} + G_{т.г} \cdot c_{т.г} \cdot \theta_{т.г} + q_r \cdot k \cdot x_b{}^m - G_{р.г} \cdot c_{р.г} \cdot \theta out_{р.г} = V_{р.г} \cdot c_{р.г} \cdot \cdot \rho_{р.г}\frac{d\theta out_{р.г}}{dt} \quad (8)$$

$$k = A \cdot e^{-\frac{E_a}{R \cdot \theta out_{р.г}}} \quad (9)$$

$$y = G_{р.г} \cdot c_{р.г} \cdot q_r \cdot A \cdot E_a \frac{e^{\frac{E_a}{R \cdot \theta out_{р.г}}}}{R \cdot \theta out_{р.г}} \quad (10)$$

$$\frac{G_{р.г} \cdot c_{р.г}}{y} \cdot \Delta\theta in_{р.г} + \frac{G_{т.г} \cdot c_{т.г}}{y} \cdot \Delta\theta_{т.г} = \frac{V_{р.г} \cdot c_{р.г} \cdot \rho_{р.г}}{y}\frac{d\Delta\theta out_{р.г}}{dt} + \Delta\theta out_{р.г} \quad (11)$$

$$k_{\theta in\_G} = \frac{G_{р.г} \cdot c_{р.г}}{y} \qquad k_{\theta out\_tg} = \frac{G_{т.г} \cdot c_{т.г}}{y} \quad T2 = \frac{V_{р.г} \cdot c_{р.г} \cdot \rho_{р.г}}{y} \quad (12)$$

Equations in canonical form

$$k_{\theta in\_G} \cdot \Delta\theta in_{р.г} + k_{\theta out\_tg} \cdot \Delta\theta_{т.г} = T2\frac{d\Delta\theta out_{р.г}}{dt} + \Delta\theta out_{р.г} \quad (13)$$

Perform the transformation of equation (13) according to Laplace

$$(T2 \cdot p + 1)\Delta\theta out_{р.г} = \frac{k_{\theta out\_tg} \cdot k_{Gair\_\theta tg}}{(T1 \cdot p + 1)}\Delta G_{пов} \quad (14)$$

$$\frac{\theta out_{р.г}(p)}{\Delta G_{пов}(p)} = \frac{k_{\theta out\_tg} \cdot k_{Gair\_\theta tg}}{(T1 \cdot p + 1)(T2 \cdot p + 1)} \quad (15)$$

According to the results of the transformations, the transfer function of the system via the control channel «air flow - the temperature of the reaction gases at the outlet» was obtained.

$$W(p) = \frac{k_{\theta out\_tg} \cdot k_{Gair\_\theta tg}}{(T1 \cdot p + 1)(T2 \cdot p + 1)} \quad (16)$$

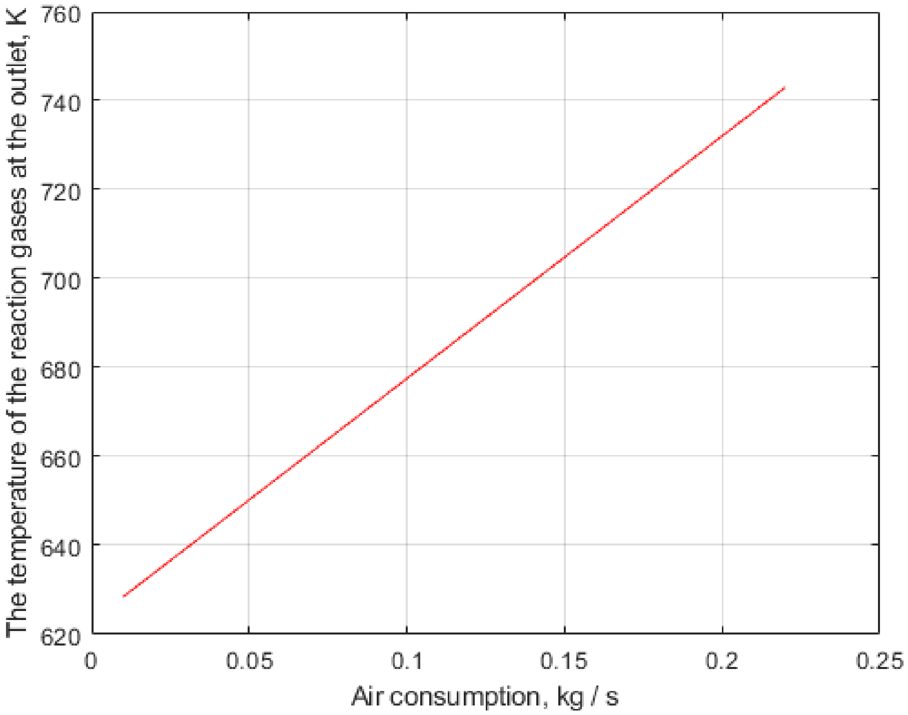

Fig. 2 Static characteristic on the channel $G_{пов} \to \theta out_{р.г}$

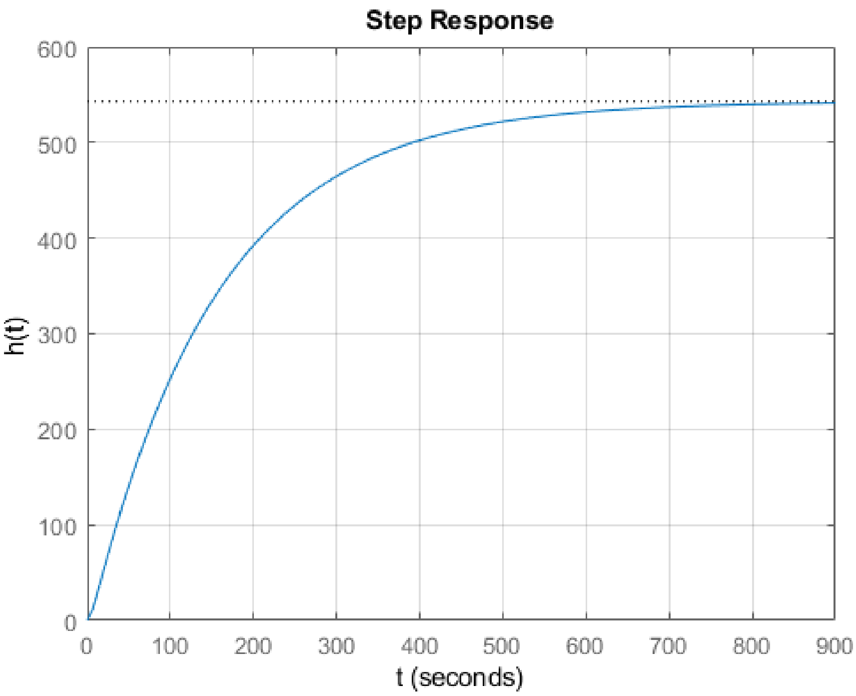

Fig. 3 Dynamic characteristic on the channel $G_{пов} \to \theta out_{р.г}$

Literature

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