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# Static optimization of methane chlorination process

**Olefir O.M. Ladieva L.R.**

*Igor Sikorsky Kyiv Polytechnic Institute, ololmkbc@gmail.com*

Chlorine derivatives have a very diverse field of application: in the production of various polymers, construction, food and textile industries.

Optimization of methane chlorination process is considered. Accepted assumptions:

- reactor walls are thermally insulated;
- the temperature of fuel and raw materials remain unchanged;
- heat capacity and density of raw materials are constant;
- this reactor is an object with concentrated parameters.

$$\begin{cases} G_{\text{р.г}} \cdot c_{\text{р.г}} \cdot \theta in_{\text{р.г}} + G_{\text{т.г}} \cdot c_{\text{т.г}} \cdot \theta_{\text{т.г}} + q_r \cdot k \cdot {x_b}^m - G_{\text{р.г}} \cdot c_{\text{р.г}} \cdot \theta out_{\text{р.г}} = 0 \\ G_{\text{п}} \cdot c_{\text{п}} \cdot \theta_{\text{п}} + \alpha \cdot G_{\text{пов}} \cdot c_{\text{пов}} \cdot \theta_{\text{пов}} - G_{\text{т.г}} \cdot c_{\text{т.г}} \cdot \theta_{\text{т.г}} = 0 \end{cases}$$

The main task in the process of methane chlorination is to maintain a given temperature inside the reactor. The air flow at the inlet to the furnace is selected as the control effect.

Table 2.1 Used notations

| Name | Designation | Numeric value | Dimension |
|---|---|---|---|
| Consumption of reaction gases | $G_{р.г}$ | 0,5 | kg/s |
| Consumption of flue gases | $G_{т.г}$ | 0,02 | kg/s |
| Fuel consumption | $G_п$ | 0,02 | kg/s |
| Temperature of reaction gases (inlet) | $\theta in_{р.г}$ | 100 | ˚C |
| Weight coefficients | q, r | 1 | - |

To solve the problem of static optimization, we chose the quadratic optimality criterion where $\theta out_{\text{р.г}_{\text{зав}}}$ - the set temperature of the reaction gases at the outlet:

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$$I = \frac{1}{2} * q\left(\theta\text{out}_{\text{р.г}} - \theta\text{out}_{\text{р.г}_{\text{зав}}}\right)^2 + \frac{1}{2} * r * \text{G}_{\text{пов}}{}^2$$

To convert the conditional optimization problem to unconditional, we used the Lagrange function, where λ1, λ2 are Lagrange factors, $G_{\text{пов}}min, G_{\text{пов}}max$ are control constraints, and the inverse penalty function was used to take into account control constraints.

$$L = \frac{1}{2}q\left(\theta\text{out}_{\text{р.г}} - \theta\text{out}_{\text{р.г}_{\text{зав}}}\right)^2 + \frac{1}{2}r \cdot \text{u}^2 + \lambda 1 \cdot (G_{\text{р.г}} \cdot \text{c}_{\text{р.г}} \cdot \theta in_{\text{р.г}} + G_{\text{т.г}} \cdot \text{c}_{\text{т.г}} \cdot \theta_{\text{т.г}} + q_r \cdot k \cdot x_b{}^m - G_{\text{р.г}} \cdot \text{c}_{\text{р.г}} \cdot \theta out_{\text{р.г}}) + \lambda 2 \cdot (G_{\text{п}} \cdot \text{c}_{\text{п}} \cdot \theta_{\text{п}} + \alpha \cdot G_{\text{пов}} \cdot \text{c}_{\text{пов}} \cdot \theta_{\text{пов}} - G_{\text{т.г}} \cdot \text{c}_{\text{т.г}} \cdot \theta_{\text{т.г}}) + k \cdot (\frac{1}{G_{\text{пов}}^{max} - G_{\text{пов}}} + \frac{1}{G_{\text{пов}} - G_{\text{пов}}^{max}})$$

Necessary conditions for optimality

$$\frac{\partial L}{\partial \theta out_{\text{р.г}}} = 0, \frac{\partial L}{\partial \theta_{\text{п}}} = 0, \frac{\partial L}{\partial G_{\text{пов}}} = 0$$

**Gradient procedure**

To find the minimum of the objective function, it was decided to choose a gradient procedure and compare it with the method of sequential quadratic programming.

$$\mathbf{G}_{\text{пов}}{}^{(\boldsymbol{k}+\mathbf{1})} = \mathbf{G}_{\text{пов}}{}^{(\boldsymbol{k})} - \boldsymbol{k}^* \cdot \frac{\boldsymbol{\partial L}}{\boldsymbol{\partial \theta out}_{\text{р.г}}{}^{(\boldsymbol{k})}}$$

**Method of sequential quadratic programming.**

This method is based on the strategy of active elections. The first step is to calculate the most probable point, the second is to create a sequence of points that most likely already coincide with the required solution.

The results of the search for minima are presented in the figures

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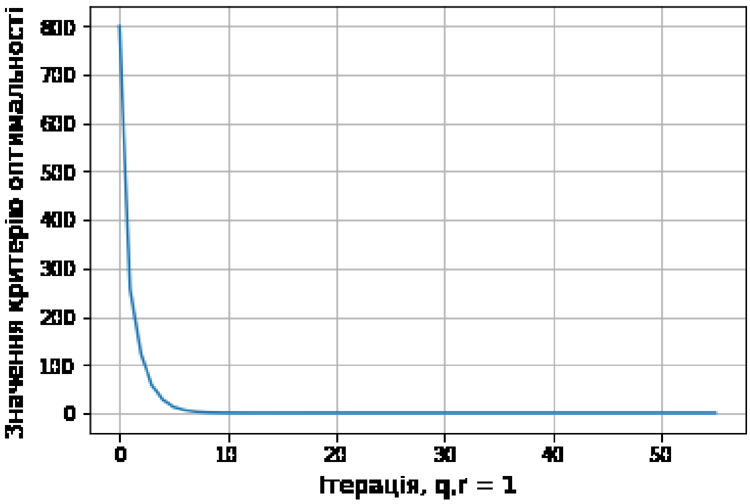


Figure 4.2 Graph of the optimality criterion depending on the iteration for the gradient procedure

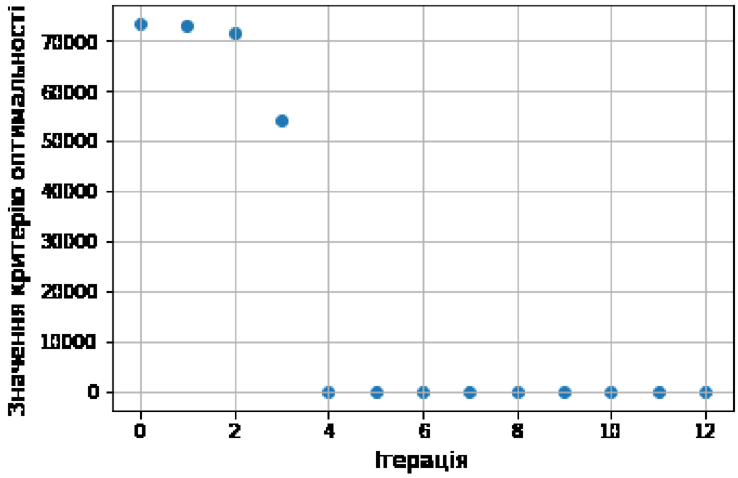


Figure 1.2. Graph of change of the optimality criterion for the method of sequential quadratic programming

The results of research have shown that the method of quadratic programming achieves results in fewer iterations and is therefore better.

## Literature

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