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AUTOMATED CONTROL OF THE HIGH-TEMPERATURE PROCESS OF ACETYLENE PRODUCTION FROM METHANE

Purpose. *A comprehensive study and improvement of automatic control systems for the acetylene production process via oxidative pyrolysis of methane. The work is aimed at solving the problem of stabilizing the yield of the target product under high-temperature synthesis conditions while minimizing energy consumption and ensuring maximum production safety.*

Methodology. *The research is based on a systematic analysis of the technological process as an automation object. Methods of mathematical modeling of chemical engineering systems (CES) were applied, including the development of static and dynamic characteristics of the reaction unit. Classical controller tuning methods (Ziegler–Nichols, M-circle) were used to optimize control parameters in combination with modern automatic tuning software tools (PID Tuner). The software implementation was carried out using an object-oriented approach to create a visual simulation environment.*

Results. *The kinetic features of oxidative pyrolysis were described in detail; a multi-criteria mathematical model of the reactor was developed, taking into account the influence of temperature and reactant ratio (oxygen/methane). Accurate models of the system's static and dynamic operating modes were created. A software product was developed that enables simulation of transient processes in the reactor, while integrated controllers ensure the stability of key parameters (temperature, pressure, and reactant composition), which are critical for achieving the desired product yield.*

Scientific novelty. *A comprehensive approach to modeling methane oxidative pyrolysis is proposed, combining analytical reactor models with modern methods of control system synthesis. A dedicated visual software interface for modeling systems with chemical reactors of this type was developed and implemented, enabling prompt response to technological process anomalies.*

Practical significance. *The analysis of the obtained results demonstrated that the modeling methods proposed in this study can be applied in industrial production, increasing raw material (methane) utilization efficiency, reducing costs, and ensuring a high level of safety through automatic prevention of emergency situations. The results contribute to the environmental sustainability and economic stability of chemical enterprises.*

Keywords: *material and heat balance; energy efficiency; engineering modeling; control system.*

Introduction. Acetylene remains a key feedstock for organic synthesis and is widely used in the production of polymers, solvents, synthetic rubber, and other valuable chemical products. In the past, the carbide method of acetylene production predominated in industry; however, it has several significant limitations, including high energy consumption, substantial CO_2 emissions, and the generation of large amounts of solid waste, which complicates its application under modern environmental and energy requirements.

A more advanced approach is the oxidative pyrolysis of methane—a process in which natural gas is partially oxidized at high temperatures over a very short residence time. Unlike the carbide method, it operates continuously, produces no solid waste, and consumes less energy. Moreover, the process is autothermal: the heat released during partial oxidation sustains the required pyrolysis temperature without additional energy input.

At the same time, the oxidative pyrolysis of methane is a high-temperature process that is highly sensitive to changes in the ratio of gas components, temperature, pressure, and the residence time of reactants in the reaction zone. Even minor deviations can reduce acetylene yield, lead to the

formation of by-products (CO, CO_2, soot), and decrease overall production efficiency. Therefore, the development of reliable automated process control systems is of particular importance.

Modern chemical industry actively integrates digital technologies, mathematical modeling, and intelligent control algorithms to enhance energy efficiency, operational stability, and environmental sustainability. The use of multi-loop control systems, adaptive and predictive control methods makes it possible to maintain optimal operating conditions of the methane oxidative pyrolysis reactor even under variable loads and external disturbances.

Thus, acetylene production by oxidative pyrolysis is the most widespread industrial-scale method, and its automation and optimization are of great economic importance. In addition, toxic and highly flammable substances are involved in this process, and their emissions into the atmosphere pose a significant threat to the global environment.

Analysis of recent research and publications. Mathematical modeling of the acetylene production process from methane is a key tool for analyzing reaction kinetics, optimizing technological parameters, and further designing automated control systems. Considering the extreme conditions of methane oxidative pyrolysis—high temperatures, short contact times, and complex multistage chemistry—several main approaches to modeling this process have emerged in the scientific literature.

Kinetic and thermodynamic modeling of methane pyrolysis. Many international studies focus on developing detailed and reduced kinetic mechanisms for the thermal decomposition of methane leading to acetylene formation. For example, the review by A. Mianowski [1] analyzes modern kinetic schemes describing the formation of C_2 hydrocarbons in the gas phase. The authors note that most models are based on systems of stiff differential equations that account for dozens or even hundreds of elementary reactions and can be used to predict acetylene selectivity depending on temperature and reactant residence time.

Further development of this direction is presented in the study "*Compact and accurate chemical mechanism for methane pyrolysis with PAH growth*" by Khrabry, [2], which proposes a compact yet sufficiently accurate kinetic mechanism for methane pyrolysis. The model successfully reproduces experimental data on acetylene formation while reducing computational costs, making it suitable for integration into optimization and automated control systems.

Reactor and numerical models of acetylene formation. In addition to kinetic approaches, significant attention has been paid to reactor modeling, particularly under the assumption of ideal plug flow (Plug Flow Reactor). In the study "*Simulation of acetylene formation from methane in a plasma jet*" by I.V. Bilera [3], a numerical model of acetylene formation from methane was implemented, taking into account both thermal and chemical effects. Although the research concerned a plasma reactor, the applied mass and heat transfer equations, as well as the kinetic approach, remain relevant to methane oxidative pyrolysis.

In numerous works devoted to high-temperature reactors, CFD models are employed to analyze spatial profiles of temperature, concentrations, and reaction rates. Such models provide a deep understanding of the process; however, due to their high computational complexity, they are rarely applied directly in real-time control systems.

Ukrainian research on mathematical modeling and automation. In Ukrainian studies, modeling of methane pyrolysis is primarily considered in the context of automated control systems. For example, in the work "*Modeling of reaction tubes of a tubular furnace in methane conversion*" by A.I. Zhuchenko and O.I. Matviienko [8], a mathematical description of a reaction tube was proposed using systems of differential equations that account for heat and material balances. Although the main focus was methane conversion, the applied methodological approach is closely related to pyrolysis problems.

Thus, the literature analysis shows that international research concentrates on detailed kinetic and numerical modeling of methane pyrolysis, ensuring a high level of physicochemical accuracy but characterized by considerable computational complexity and limited suitability for real-time control applications. In contrast, Ukrainian studies are oriented toward engineering modeling and practical automation. At the same time, the issue of integrating adequate mathematical models of methane oxidative pyrolysis with modern automated control algorithms remains insufficiently explored, which limits the possibilities for real-time process optimization.

In view of this, it is relevant to develop a mathematical model of acetylene production by methane oxidative pyrolysis that combines an adequate description of the main physicochemical patterns with acceptable complexity for further use in automated control systems. Such a model should reflect the dynamics of the temperature regime, the influence of reactant ratios, and the residence time of the gas mixture in the reaction zone on the yield of the target product.

Accordingly, this work presents a mathematical description of the methane oxidative pyrolysis process based on material and heat balances of the reaction zone. The proposed model is used as a basis for analyzing the dynamic properties of the control object and substantiating the structure of the automated control system.

Materials and Methods. The key unit in the methane oxidative pyrolysis process is the pyrolysis chemical reactor, since its operating conditions directly determine the degree of methane conversion into acetylene. The process occurring in the reactor can be divided into three main stages: mixing, pyrolysis, and quenching.

Mixing is the process of forming a gas mixture of methane and oxygen supplied to the reactor inlet.

Pyrolysis is a cascade of chemical reactions that determines the final concentration of acetylene and other products. Each reaction in this cascade affects the composition of the gas mixture and the overall selectivity.

Quenching is the heat exchange process between the pyrolysis products and water separately introduced into the reactor, which ensures temperature control and stabilization of the reaction products.

Problem Statement of Modeling. Among all stages of the process, the acetylene concentration is directly influenced by the cascade of pyrolysis chemical reactions, which defines the control object. The selected control variable is the contact time of the reactants in the reaction zone (τ), as it directly affects the degree of methane conversion.

The controlled output variable is the acetylene concentration at the outlet of the reaction zone ($C_{(}C_2H_{2)}$). Reaction parameters such as the rate constants of methane decomposition (k_3) and acetylene decomposition (k_4) cannot be directly regulated and are considered system disturbances.

The structural-parametric diagram of the reaction zone of the methane pyrolysis reactor is shown in Fig. 1.

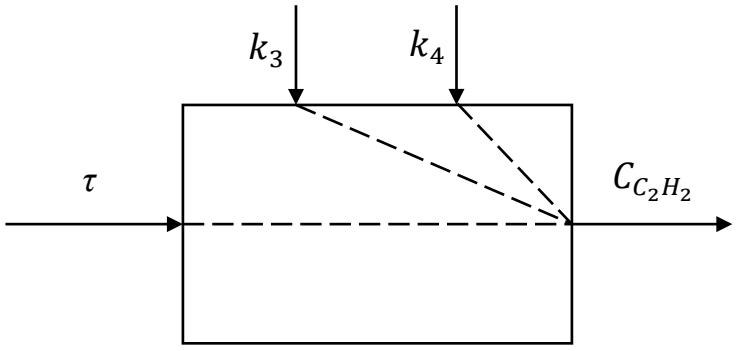


Figure 1. **Structural-parametric diagram of the reaction zone of the pyrolysis reactor**

Thus:

- ***Determining parameter*** – acetylene concentration at the reactor outlet, $C_{(}C_2H_2)$.
- ***Control action*** – contact time of reactants in the reaction zone, τ.
- ***Disturbances*** – rate constant of methane decomposition to acetylene, k_3; rate constant of acetylene decomposition, k_4.

Results and Discussion. The material balance of the chemical reactor is represented by a system of equations describing the concentrations of each chemical species participating in the reactions occurring within the reactor. In the methane oxidative pyrolysis reactor, four reactions take place simultaneously.

At the oxidation stage, methane and oxygen react with heat release according to the following equations:

$$CH_4 + O_2 \overset{k_1}{\rightarrow} CO + H_2 + H_2O - \Delta H, \Delta H = 272 \text{ kJ/mol};$$
$$CH_4 + 2O_2 \overset{k_2}{\rightarrow} CO_2 + 2H_2O - \Delta H, \Delta H = 891 \text{ kJ/mol}.$$

The heat released during combustion is used for the pyrolysis of the unreacted methane according to the reaction:

$$2CH_4 \overset{k_3}{\leftrightarrow} C_2H_2 + 3H_2 + \Delta H, \Delta H = 376 \text{ kJ/mol}.$$

Subsequently, the formed acetylene continues to decompose under the influence of heat according to the reaction:

$$C_2H_2 \overset{k_4}{\leftrightarrow} 2C + H_2 + \Delta H, \Delta H = 227.4 \text{ kJ/mol}.$$

For each unique species, an equation of the following general form is written:

$$\frac{1}{\tau}(C_A^{\text{вх}} - C_A) = \pm k_A C_A,$$

where τ – is the reactant residence time in the reaction zone; C_A^{in} –is the inlet concentration of component; A, C_A – is its concentration in the reactor; k_A – is the corresponding reaction rate constant.

Material Balance.

$$\begin{cases} \frac{1}{\tau}\left(C_{CH_4}^{\text{вх}} - C_{CH_4}\right) = k_1 C_{CH_4} C_{O_2} + k_2 C_{CH_4} C_{O_2}^2 + 2k_3 C_{CH_4}^2 \\ \frac{1}{\tau}\left(C_{O_2}^{\text{вх}} - C_{O_2}\right) = k_1 C_{CH_4} C_{O_2} + 2k_2 C_{CH_4} C_{O_2}^2 \\ \frac{1}{\tau}(C_{CO}^{\text{вх}} - C_{CO}) = -k_1 C_{CH_4} C_{O_2} \\ \frac{1}{\tau}\left(C_{CO_2}^{\text{вх}} - C_{CO_2}\right) = -k_2 C_{CH_4} C_{O_2}^2 \\ \frac{1}{\tau}\left(C_{H_2}^{\text{вх}} - C_{H_2}\right) = -k_1 C_{CH_4} C_{O_2} - 3k_3 C_{CH_4}^2 - k_4 C_{C_2H_2} \\ \frac{1}{\tau}\left(C_{H_2O}^{\text{вх}} - C_{H_2O}\right) = -k_1 C_{CH_4} C_{O_2} - 2k_2 C_{CH_4} C_{O_2}^2 \\ \frac{1}{\tau}\left(C_{C_2H_2}^{\text{вх}} - C_{C_2H_2}\right) = -k_3 C_{CH_4}^2 + k_4 C_{C_2H_2} \\ \frac{1}{\tau}(C_C^{\text{вх}} - C_C) = -2k_4 C_{C_2H_2} \end{cases}.$$

Heat Balance:

$$\frac{1}{\tau}(T_{\text{вх}} - T) = -\frac{k_1 C_{CH_4} C_{O_2} Q_1 + k_2 C_{CH_4} C_{O_2}^2 Q_3 + k_3 C_{CH_4}^2 Q_3 + k_4 C_{C_2H_2} Q_4}{p C_p}.$$

Table 1

Steady-State Parameters

Parameter	Symbol	Value	Units
Reactant contact time	**τ**	0.005	c
Oxygen concentration at the outlet of the reaction zone	C_{O_2}	4.4e-4	kg/m³
Acetylene concentration at the inlet of the reaction zone	$C_{C_2H_2}^{\text{вх}}$	0	kg/m³
Methane concentration at the outlet of the reaction zone	C_{CH_4}	0.0133	kg/m³
Rate constant of methane decomposition to acetylene	k_3	1.414e7	c^{-1}
Rate constant of acetylene decomposition	k_4	6053.2	c^{-1}

Based on the tabulated values, the transfer function coefficients are calculated as follows:

$$C_{C_2H_2}(\tau, k_3, k_4) = \frac{k_3 \tau C_{CH_4}^2 + C_{C_2H_2}^{\text{вх}}}{k_4 \tau + 1} = \frac{0.0133^2 \text{k}_3 \tau}{k_4 \tau + 1}.$$

Static Characteristic for $C_{C_2H_2}(\tau) = f(\tau)$: (Fig. 2).

$$C_{C_2H_2}(\tau) = \frac{25.0122\tau}{6053.2\tau + 1}.$$

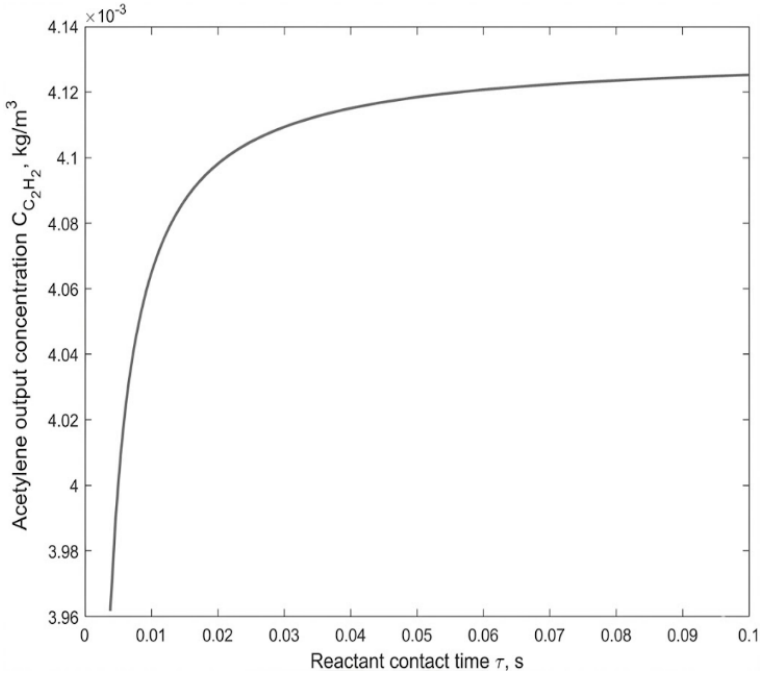


Figure 2. **Static characteristic for the "control" – "output" channel**

Static characteristic for $C_{C_2H_2}(k_3) = f(\text{k}_3)$:

$$C_{C_2H_2}(k_3) = 2.8288\text{e} - 10k_3.$$

Static characteristic for $C_{C_2H_2}(k_4) = f(k_4)$: plots of the static characteristics for f(k3) (Fig. 3a) and f(k4) (Fig. 3b), respectively.

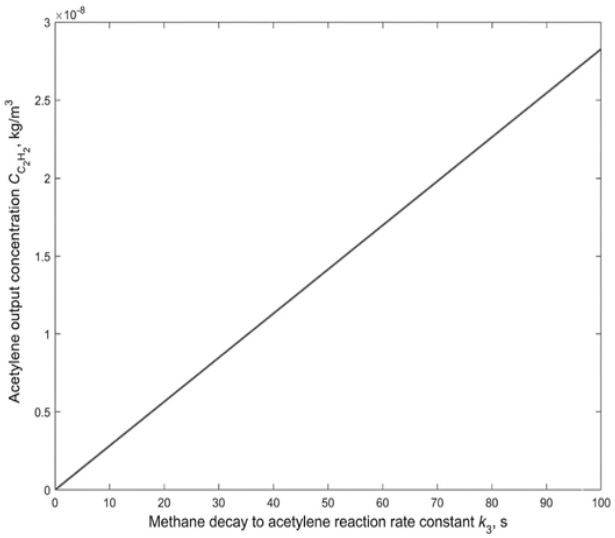


Figure 3a. **Static characteristic for the "disturbance No.1" – "output" channel**

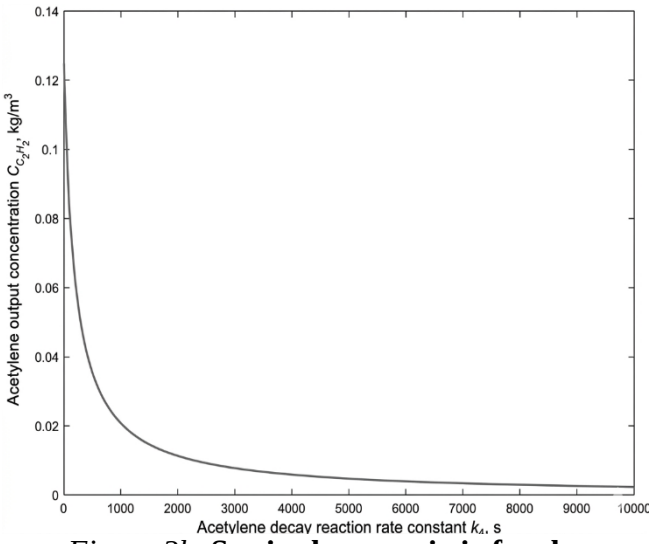


Figure 3b. **Static characteristic for the "disturbance No.2" – "output" channel**

Simulation of the Dynamic Mode.

The dynamic equation has the following form:

$$\frac{d\boldsymbol{C}_{\boldsymbol{C_2H_2}}(\boldsymbol{t})}{\boldsymbol{dt}} = \frac{\mathbf{1}}{\boldsymbol{\tau(t)}}\left(\boldsymbol{C}^{\text{вх}}_{\boldsymbol{C_2H_2}} - \boldsymbol{C}_{\boldsymbol{C_2H_2}}(\boldsymbol{t})\right) + \boldsymbol{C}^{\mathbf{2}}_{\boldsymbol{CH_4}}\boldsymbol{k_3(t)} - \boldsymbol{k_4(t)C_{C_2H_2}(t)}.$$

Linearized equation:

$$\frac{d}{dt}\Delta C_{C_2H_2}(t) + \left(k_4 + \frac{1}{\tau}\right)\Delta C_{C_2H_2}(t) = \frac{C_{C_2H_2} - C^{\text{вх}}_{C_2H_2}}{\tau^2}\Delta\tau(t) + {C_{CH_4}}^2\Delta k_3(t) - -C_{C_2H_2}\Delta k_4(t);$$

$$f_2(t) = \frac{\Delta k_4(t)}{k_4} \rightarrow \Delta k_4(t) = k_4 f_2(t).$$

Laplace Transform (with respect to time)

$$\left(C_{C_2H_2}s + C_{C_2H_2}\left(k_4 + \frac{1}{\tau}\right)\right)y(s) = \frac{C_{C_2H_2} - C^{\text{вх}}_{C_2H_2}}{\tau}u(s) + {C_{CH_4}}^2 k_3 f_1(s) - -\left(C_{C_2H_2}k_4\right)f_2(s).$$

After introducing the notations:

$$K_1 = -k_4 = -6053;\ K_2 = \frac{{C_{CH_4}}^2 k_3}{C_{C_2H_2}} = 6253;$$

$$K_3 = \frac{C_{C_2H_2} - C^{\text{вх}}_{C_2H_2}}{C_{C_2H_2}\tau} = 200;\ T_1 = \frac{k_4\tau + 1}{\tau} = 6253.$$

We obtain the canonical form:

$$y(s) = \frac{K_1}{T_1 s+1}f_2(s) + \frac{K_2}{T_1 s+1}f_1(s) + \frac{K_3}{T_1 s+1}u(s).$$

Transfer Functions:

Control channel $u(s) \to y(s)$:

$$W_1(s) = \frac{y(s)}{u(s)} = \frac{K_3}{T_1 s + 1} = \frac{200}{6253s + 1}.$$

Disturbance channel $f_1(s) \to y(s)$:

$$W_2(s) = \frac{y(s)}{f_1(s)} = \frac{K_2}{T_1 s + 1} = \frac{6253}{6253s + 1}.$$

Disturbance channel $f_2(s) \to y(s)$:

$$W_3(s) = \frac{y(s)}{f_2(s)} = \frac{K_1}{T_1 s + 1} = \frac{-6053}{6253s + 1}.$$

Overall System Transfer Function:

$$W(s) = W_1(s) + W_2(s) + W_3(s).$$

We will construct the step responses for all channels.

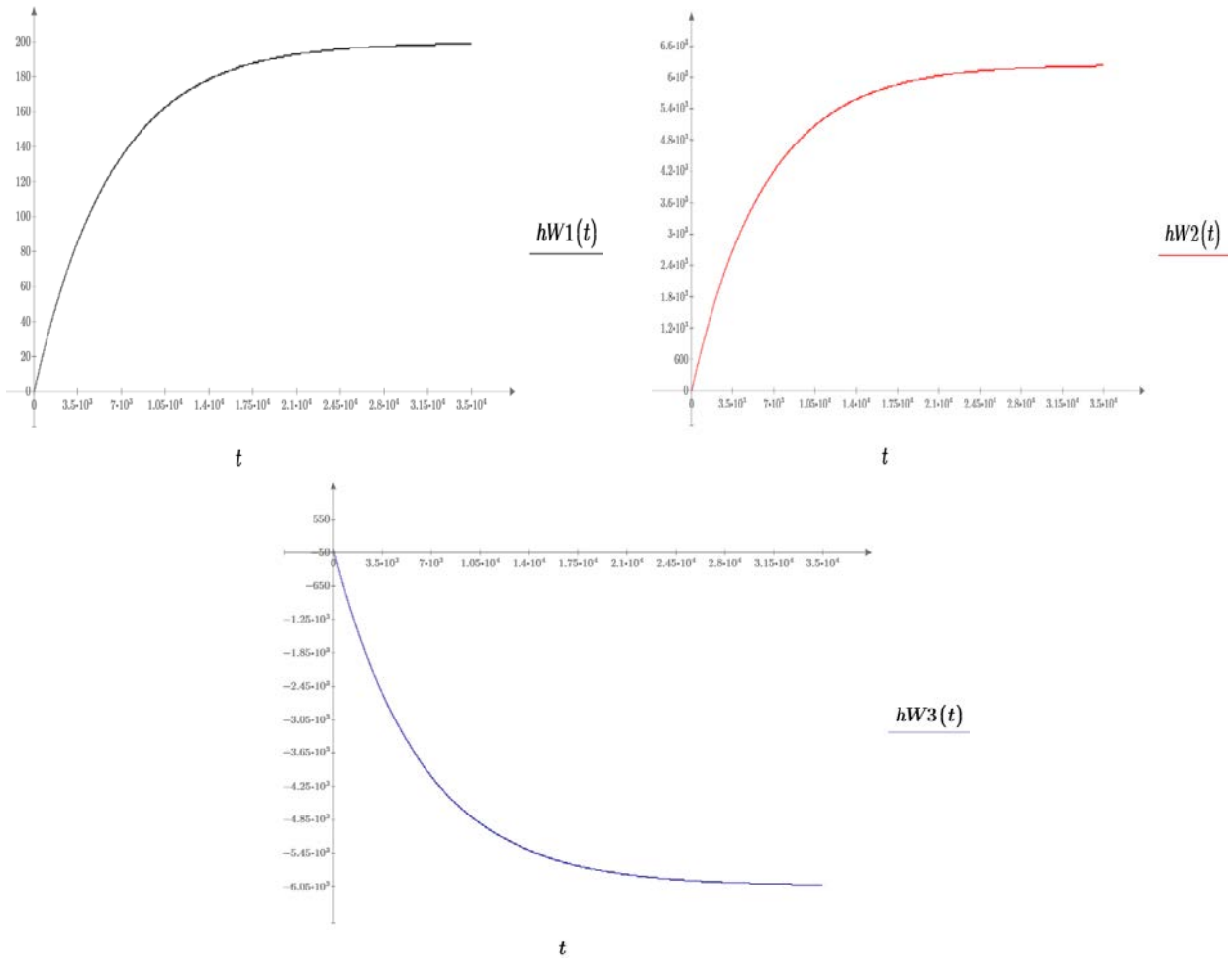


Figure 4. **Step responses for all control channels**

Visual Representation of the Script and Interfaces. For the process of modeling and synthesizing the control system of the oxidative pyrolysis chemical reactor, application software was

developed. Using a simple and intuitive visual interface, it allows the user to influence the process and analyze the results.

In this work, the MATLAB executable file format – ***Live Script*** – was used to create the software product.

Thanks to the ***Symbolic Math Toolbox*** add-on, all equations and related calculations can be fully automated. In addition, the static-mode parameters are entered through numeric input fields, and based on them, the static characteristic is constructed.

The parameters of the static mode, previously entered by the user, are substituted into the derived transfer function formulas. The symbolic equations are then converted into transfer functions using the ***Control System Toolbox*** add-on in MATLAB. This same toolbox makes it very easy to construct step responses.

A controller and feedback are required for system control. A PID controller (Proportional–Integral–Derivative controller) was selected and tuned.

Several methods were used to tune the PID controller parameters:

- Ziegler–Nichols tuning method;
- M-circle method;
- PID Tuner (PID-Tune).

The PID-Tune method proved to be the most effective.

The built-in MATLAB PID tuning method uses its own iterative search algorithm. Unlike the previous methods, it allows automatic determination of the parameters for any type of PID controller.

In addition to the code, the script page can also include the corresponding calculation formulas and explanations of the processes taking place.

Comparison of the Obtained Controllers. To compare the controllers, the following set of system performance criteria (for the systems to which they were added) is considered:

- Settling time
- Overshoot
- Stability margin
- Integral squared error (ISE)

All calculations are performed using built-in MATLAB functions. The values of settling time and overshoot are obtained using the stepinfo() function.

The stability margin is defined as the largest value of the real part of the system poles obtained using the pole() function.

The integral squared error of the system over the interval [t0;tn][t_0; t_n][t0;tn] is calculated using the following formula:

$$I_0 = \int_{t_0}^{t_n} \big(r(t) - y(t)\big)^2 dt.$$

Table 2

Comparison of the developed control systems

Controller tuning method	Settling time, s	Overshoot, %	Stability margin	ISE
Ц-Н (П)	17803.23	0	3.431445e-4	5534.658
Ц-Н (ПІ)	132283.2	0	3.601906e-5	5326.153
Ц-Н (ПІД)	55408.84	0	1.054670e-4	2322.181
М-коло (ПІ)	2.548416e-5	31.1	159918.1	1.567e-6
PID-Tune (П)	6.109081e-6	0	1000000	5.014e-7
PID-Tune (ПІ)	1.068558e-5	24.3	433012.7	5.839e-7
PID-Tune (ПІД)	1.786645e-5	2.5	30375.54	5.008e-7

From Table 2, it can be seen that the system tuned using ***PID-Tune*** with a P-controller performed the best.

Although a higher gain could have been selected for the controller tuned using the M-Circle method during the calculation process, this would not have eliminated the overshoot. Therefore, regardless of the gain value, the resulting controller would still have been inferior to the one generated by PID-Tune.

The only criterion in which the P-controller was slightly inferior to the PID-controller was the integral squared error (ISE). However, the difference is so small that it can be neglected.

In addition to the code, the script page can also include the corresponding calculation formulas and explanations of the processes that take place.

Controller Tuning (PID-Tune):

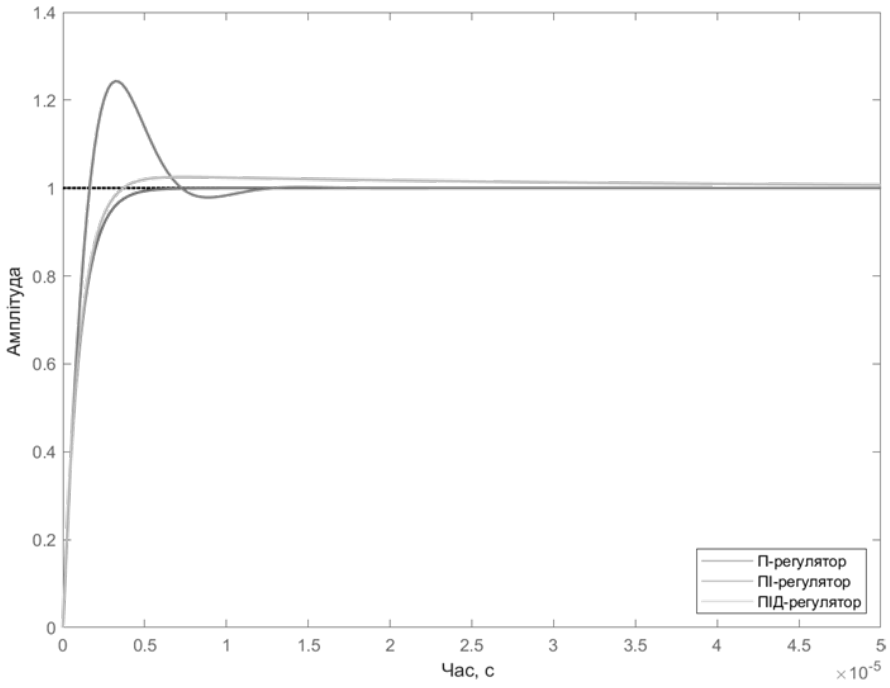
Controller tuning using the built-in *pidtune* function.

Speed–stability trade-off (wc): 1000000
Phase Margin: 60
Design Focus: reference tracking
Number of Unstable Poles (NumUnstablePoles): 0

P-controller parameter: K_P = 31266000

PI-controller parameters: K_P = 2.707715e+07, TI=1.732051e−06

PID-controller parameters**:** K_P = 3.125254e+07, TI=3.395312e−05, T_I = 3.395312e-05, T_D = 9.999971e−11



settling time - 6.109081e-06
overshoot - 0.0%
stability margin - 1.000000e+06
ISE = 5.014124e-07

Figure 4. **Presents a fragment of the interface for tuning controller parameters using the PID-Tune system**

Conclusion. In this work, an analysis of the acetylene production process by means of oxidative pyrolysis of methane was carried out.

Using the equations of the mathematical model and the transfer functions developed in this study, a computer simulation of the reactor operation was performed, and its response to various input values and disturbances was evaluated.

Based on this model, a control system with a controller was synthesized, and its optimal parameters were programmatically tuned without requiring access to the real plant.

The created visual interface made it possible to easily and conveniently investigate the process of modeling and control system synthesis for the oxidative pyrolysis of methane process.

The presented script is only a simple example of what can be achieved using the Live Script format, but it can be easily adapted to any other process that requires automation.

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АВТОМАТИЗОВАНЕ КЕРУВАННЯ ВИСОКОТЕМПЕРАТУРНИМ ПРОЦЕСОМ ОДЕРЖАННЯ АЦЕТИЛЕНУ З МЕТАНУ

Мета. *Комплексне дослідження та вдосконалення систем автоматичного керування процесом отримання ацетилену методом окислювального піролізу метану. Робота спрямована на розв'язання задачі стабілізації виходу цільового продукту в умовах високотемпературного синтезу та мінімізацію енергоресурсів при забезпеченні максимальної безпеки виробництва.*

Методика. *В основу дослідження покладено системний аналіз технологічного процесу як об'єкта автоматизації. Використано методи математичного моделювання хіміко-технологічних систем (ХТС) з розробкою статичних та динамічних характеристик реакційного вузла. Для оптимізації параметрів керування застосовано класичні методи налаштування регуляторів (**Циглера-Нікольса**, **М-кола**) у поєднанні з сучасними програмними інструментами автоматичного тюнінгу (**PID-Tuner**). Програмна реалізація виконана з використанням об'єктно-орієнтованого підходу для створення візуального середовища моделювання.*

Результати. *Детально описано кінетичні особливості окислювального піролізу; розроблено багатокритеріальну математичну модель реактору, що враховує вплив температури та співвідношення реагентів (кисень/метан). Розроблено точні моделі статичних і динамічних режимів роботи системи. Створено програмний продукт, що дозволяє проводити імітаційне моделювання*

перехідних процесів у реакторі, а інтегровані регулятори забезпечують стабільність параметрів (температури, тиску, складу реагентів), що критично для виходу цільового продукту

Наукова новизна. *Запропоновано комплексний підхід до моделювання окислювального піролізу метану, що поєднує аналітичні моделі реактору з сучасними методами синтезу систем керування. Розроблено та реалізовано програмний візуальний інтерфейс для специфічного моделювання систем з хімічними реакторами цього типу, що дозволяє оперативно реагувати на аномалії техпроцесу.*

Практична значимість. *Аналіз отриманих результатів показав, що методи моделювання, запропоновані в цій роботі, можуть бути використані на промисловому виробництві, що дозволяє підвищити ефективність використання сировини (метану), знизити витрати та забезпечити високий рівень безпеки через автоматичне запобігання аварійним ситуаціям. Отримані результати сприяють екологічній стійкості та економічній стабільності хімічних підприємств.*

Ключові слова: *матеріальний та тепловий баланс; енергоефективність; інженерне моделювання; система керування.*