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HIGHER EDUCATION FUNDING IN IRAQ IN TERMS OF THE EXPERIENCE OF PARTICULAR DEVELOPED COUNTRIES

Atiya Abbas Gatea, Vrazhnova M.

Education funding is considered to be one of the issues that quite a few universities around the world have been preoccupied with as it is the basic element to fulfil their goals in this field.

Education expenditures clearly show how important education is thought to be in a particular country. This is an ongoing issue since it is related to changes in the global economy system and the increase in education expenditures in general and of higher education in particular, that, of course, affects the level of funding from the general budget of the country.

Keywords: *funding; funding sources; funding solution.*

Introduction

The issue of funding optimization of education in general and of higher education in particular is one of the major ones that a lot of countries around the world have to face regardless of the level of their economic development. In general, funding can be defined as a certain amount of funds designed to be spent to perform a specific job in order to achieve the desired economic, social or cultural goal or all of them combined.

From an administrative point of view funding can be described as an administrative duty that implies financial planning in order to obtain the funds from the relevant sources to provide for particular financial requirements and ensure an organization's continuous activity.

University funding can be defined as a combination of financial resources allocated for the university education from the general budget of the country as well as a number of other sources, such as donations, tuition fees, domestic and international grants by various organizations and foundations, economic activity revenues, loans.

The conventional view of education funding for is none other but receiving the funds and their use to implement and develop various projects. It is mainly focused on determining the best source of funding from a number of possible ones.

At the moment, higher education in Iraq is facing certain difficulties while building up the resource support for the universities. But that is not the most significant thing. The country's existing approaches to financing are thought to be quite conservative. Thus, the financial mechanism should be built up that could combine conventional methods with non-conventional ones that take into account the funding model of the developed countries' higher schools.

Kinds of funding

The researchers of higher education financing have distinguished the following types of universities funding:

- budgetary funding;
- educational loans;
- educational services export;
- provision of material-and-technical services aimed at collecting funds;
- state registered financial obligations in the field of education;
- grants and programs;
- external funding through a system of both international and regional financial institutions, such as the International Monetary

Fund or the International Bank for Reconstruction and Development, as well as some other regional organizations in addition to the international funding programs which are presented in the form of subsidies and investments, for example, the Media program[1], started by the European Union within the framework of the Euro-Mediterranean partnership[2].

The higher education funding sources are as follows:

1. Governments

The observational studies carried out by international organizations in many countries around the world have shown that there are three models of higher education system funding on the basis of total revenues:

1. Funding received from the central government.
2. Funding received from both the central government and local authorities.
3. Funding received through cooperation between the central government, regional and local authorities.

2. Students

Students are the primary users of the learning process and, therefore, they are the most important sources of university funding in many countries around the worlds, including the developed ones. The most important funds inflow from the students are as follows:

[1] The media cooperation program, started by the European Union to assist in activities of some Arab countries the EU has partnership relations with (import, export, etc.). According to this program Egypt received a total of 352.2 (mln. EUR) in 2000–2006, Majdi Bilal, the European Union strategy towards the countries of the Southern Mediterranean region.

[2] The Euro-Mediterranean partnership – the process of state-to-state cooperation, started in 1995 between the European Union and the North African Mediterranean and West Asian countries, aimed at strengthening economic ties.

A) *The tuition fee*. This system is introduced in most developed countries as well as some developing countries. Recently, they have been joined by the Arab countries, despite the fact that it has caused a lot of resistance within these countries, where the free form of education was widespread.

B) *Student loans*. A student pays for their university education through loans obtained while they are studying. Ways and means of paying these funds back might be different in these countries.

C) *Studies bonds*. A bond is a voucher that enables one to buy some particular services. The bonds system intensifies competition between higher education institutions and makes them take greater responsibility for the quality of education provided. Study bonds. A bond is a voucher that gives the opportunity to buy some educational services. bond system intensifies competition between higher education institutions and forces them to take greater responsibility for the quality of education provided.

3. Universities

Through self-funding, making funds on their own. In this case, universities have the right to manage their financial resources in their sole discretion, not according to the rules defined by the state budget. This allows universities to engage in other activities in addition to the primary ones, that helps them earn additional funds, making it possible to finance certain activities. Thus, universities become production centres, implement research results; provide advisory services, buy and rent plots of land, buildings, etc.

4. Grassroots fundraising

The most important of these models are:

- grants and donations;
- trade unions and non-government organizations;
- alumni communities;

1. External funding

In many developing countries, university funding is based on loans coming from abroad as well as and assistance from outside. Such international institutions and organizations as the World Bank, the European market, UNESCO, etc. provide interest-free, long-term and easy-to-pay loans. However, this process needs careful studying to avoid unnecessary costs and financial losses, on the one hand, and, on the other hand, one should find out about the positive and negative sides of the proposed loan to make sure there is no secret criminal purpose of the external foreign-funding of higher education system.

Sources of higher education funding in Iraq and some Arab countries

The responsibility for the educational, research and other educational activities funding in Iraq was taken completely by the state, in particular prior to the introduction of legislation allowing the establishment of private universities and the implementation of new technologies in the field of higher education (the parallel education and e-learning). It is the government that transfers the required funds out of the state budget for universities and other educational institutions by means of the current budgetary allocations, investment tax credits. The state monitors their yearly increasing, as the rise in the number of students and the average level of applicants implies a corresponding increase in investment from the state budget in the field of higher education, if its quality and decent educational training level need to be preserved. The Japanese experience of investing in the education sector in order to accelerate the economic development of the country is the most significant evidence of the role of these institutions. The last decade saw wide introduction of private funding in the country considered as one of the main sources of education funding; as a result, in addition to the state-funded educational institutions there appeared organizations with mostly private funding.

Table 1.

Pct. comparison of the funds allocation for higher education in some Arab countries within 2008–2012.[3]

State	Year	Allocations	
		GDP pct.	State allocations pct.
Tunisia	2010	2.6	5.21
Algeria	2008	3.4	3.20
Saudi Arabia	2008	6.5	3.19
Syria	2009	1.5	7.18
Oman	2009	3.4	-
Morocco	2009	4.5	7.25
Egypt	2008	8.3	9.11
Iraq	2012	5.3	11

In Iraq, as in most Arab countries, the state continues to be the main source of education funding. In recent years, there was an increase in the amount of education funding in Iraq: government allocations rose from 6.8% in 2008 to 11% in 2012, though it is still quite low if compared with other Arab countries. According to the data provided by UNESCO (Table 1), allocation of funds for education in relation to a country's GDP (2008–2012) varies between 2.6% and 5% in Tunisia, Saudi Arabia and Yemen, whereas it amounts to 5.3% in Iraq. But in Morocco and Egypt investment in education exceeds the one in Iraq (for example, the government in Morocco allocates over 7% in the education sector). With regard to foreign countries, according to the annual report of the Organization for European Cooperation and Development (OECD) 4.7% is allocated to education in the United States, 2.7% in South Korea, whereas in Belgium, Denmark and France this ratio varies between 2.7% – 6% and 1.4% in Turkey.

Conclusion

Every country in the world carries out its economic policy and makes every effort to implement it in order to ensure the popula-

[3] UNESCO Institute for statistics, UNESCO, Paris.

tion's well-being. Its implementation is done in the form of projects designed to meet the needs and financial capabilities of the country. Funding can be characterized as the blood streaming in the veins of the project. Therefore, it can be stated that funding plays a significant role in the country's development policies and is implemented as follows:

1. Capital provision to carry out project activities that:

- provide new jobs that reduce the number of the unemployed;
- contribute to the economic development of the country;
- contribute to the fulfilment of economic goals set by the state.

2. Funding provides the well-being of the society by enhancing their subsistence level (housing, jobs provision, etc.).

Taking the above-mentioned facts as the base we can briefly introduce both positive and negative consequences of the higher education sector state and private funding, as well as try to present solutions to the problems that might be encountered.

– Education sector state funding

Advantages

- The financial barriers get eliminated to people who want to get an education (that leads to the increase in the number of educated people as well as there appears an opportunity to carry on with education).
- It is considered to be an effective means for the promotion of affordable universal education.
- It contributes to meeting the public requirements to provide compulsory education.
- It enables talented young people to carry on with their education.
- It ensures a smooth transition of professionals into various sectors of economic and social activities.
- It ensures quantity and quality workforce planning.
- It contributes to scientific and technological progress.

- It helps optimize the number of students in each field of study.

Disadvantages

- Insufficient economic motivation or its total lack that would enhance the effectiveness of education on the part of both students and teachers.
- The current system does not provide the motivation that would make it possible to enhance the university lecturer impact, as they are aware of the fact that any additional effort is unable to increase their material wealth.
- Educated personnel brain drain.
- Students and teachers are not eager to meet the educational standards.

Problem solution

- The student must bear some minor expenses, such as buying books and stationery.
- The student should pay the education costs if they fail to meet the educational requirements.
- The student should be denied a scholarship if they fail to show good academic results, just as it is done in Russia.
- The student should pay for their second and third attempts while taking an exam.
- Better opportunities should be provided for gifted students to develop their professional and scientific abilities.

– Education sector private funding

Advantages

- It provides economic incentives in the field of education and, as a result, it reduces the professional personnel brain drain.
- It stimulates the student to put more effort to achieve the effective use of educational material.

- It makes the student to carefully choose the kind of education that best fits their capabilities and expectations.
- It is an important factor for improving the quality of the student's studying in order to maximize the use of the acquired knowledge in practical life.

Disadvantages

- It creates certain financial hindrances to getting education and its further continuation.
- It makes it difficult for promising young people to get access to education.
- It limits the employees training and retraining possibilities.
- It fails to provide sufficient opportunities for the development of all branches of knowledge required by society (primarily, basic sciences).

Problem solution

- There should be a specific system based on the student's participation in the education funding aimed at creating their sense of responsibility.
- Tuition fees should be reduced for students who are having financial constraints but are characterized by their high academic potential; this should take effect after they have passed their exams to provide an incentive to enhance their scientific activity.
- Students should be given an opportunity to get an off-hour job at their university.
- There should be a selection of funding sources that will not directly or indirectly affect the quality of education.

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EMPLOYEES COMPETITIVENESS ASSESSMENT ON INTERNAL AND EXTERNAL LABOUR MARKETS

Ismailova T., Ismailov R.

This paper presents an overview of foreign and domestic research to the approaches of employees assessment in terms of their competitiveness. Based on the experience of large industrial enterprises the dominant elements that form employee competitiveness were determined. A different methodology that takes into account the impact of economic globalization was given. Its validity is based on mathematical calculations and use of software.

Keywords: *employees competitiveness (CPT); economic globalization; assessment; labour market.*

Introduction

In the process of workers' formation and development it is necessary to understand, what is formed and what is developed, what level this or that element has and what level it should have to make a worker be competitive.

In the internal labor market workers assessment allows enterprises to reveal employees strengths and weaknesses. According to the assessment results some recommendations to improve the quality and increase the employees competitiveness and goods/services can be offered.

It's assumed that various authors have their own opinion in considering the assessment of employees competitiveness (CPT). Therefore, we have identified and grouped into common approaches these definitions in chronological order.

1) 1996–2007 – labour force quality (N. Lyapkina, E. Bogdanova, L. Ivanovskaya and N. Suslova, L. Milyaeva, E. Saruhanov and S. Sotnikov, R. Fatkhutdinov);
2) 2002–2008 – the level of employees competitiveness (P. Kravtsevich, E. Galuzo, Soldatos G.);
3) 2006–2010 – systematic approach (S. Sotnikov, N. Romashkin);
4) 2010 – goal-setting in the enterprise management (E. Andrianova);
5) 2013–2015 – situational approach (T. Ismailova (Terehova) [1].

These approaches, having their evolution, were closely associated with the approaches in management as it's seen from chronological order.

These approaches may be applied at national, regional and enterprise level, because they allow to assess the efficiency of competitiveness management and the degree of implementation of the strategy for the competitiveness management. However, the performance criteria, i.e. maximum achieved with the help of competitiveness, should be defined in the program strategy.

We believe that the level of employees competitiveness, as a specific value of the competitiveness elements, can have a different demand on the internal or external labour markets, i.e. the level of competitiveness of a particular employee may be sufficient in the domestic labour market and not in demand on the external one.

We consider that the level of employees competitiveness should be understood as specific characteristics and requirements of external or internal market for it in terms of competitiveness.

The experiment

They are employers' representatives who, in a greater degree, evaluate employees competitiveness. In this case the main market motivators of employees competitiveness are the demand for this category of workers in a particular labor market and supply from the economically active population with in-demand specialties.

Competitiveness provides certain benefits to the employee, and not only him. Firstly, if an employee is competitive, he or she can easily occupy a vacant post in other enterprises or displace another worker. Secondly, if employees are competitive, Russian companies have the opportunity to compete for the leadership on the international market.

After analyzing the works of domestic and foreign authors (M. Feonova, A. Selyutina, E. Bogdanova, E. Galuzo, L. Ivanovskaya and N.A. Lyapkina, I. Suslova, T. Khlopova, I. Durakova and A. Kibanov, H. Gorelov), experts in the field “headhunting” and experience of PJSC “Novolipetsk Metallurgical Plant”, PJSC “Severstal”, PJSC “MMC “Norilsk Nickel”, we determined that the structure and content of the criteria-based elements that form the employee competitiveness, depends on many factors: the purpose of formation, the specification and requirements of the post (labour market level, industry, etc.); the employee’s field (external, internal labour markets), etc. [1]

The main drawback of the studied methods of assessment is one-sided object assessment. There are no systemic and situational approaches to the employee competitiveness assessment, taking into account the integration with the competitiveness objects and labour markets. Besides, the authors do not consider the impact of economic globalization, when the elements should be standardized for all employees.

In the conditions of economic globalization the worker will be competitive if he or she has sufficient set of elements that form economy. For example, in Soviet-type economic planning such element as higher education made a worker competitive. However, in conditions of constant spatial economic transformation it is not enough.

Thus, as the basis of the method of determining the content and level of development of the elements which form a competitive employee the following sequence of stages was given:

1) to combine all the studied elements in a single list and work out the elements-based questionnaire;

2) to poll workers to identify elements that have the greatest impact on achieving results in their professional activities, larger salaries, promotion, etc.;
3) to put the results into MS Excel (each characteristic in the survey was estimated by respondents from 0 to 100 points);
4) to process the results using software STATISTICA6;
5) to hold experts scoring (to determine the level of the development of each item and overall level);
6) to carry out the calculation with application of the formula;
7) to rank the coefficients;
8) to determine the level of employee competitiveness.

Results and discussion

On the basis of critical understanding of the methodologically accumulated base and of the analysis of requirements to the quality of the workforce and professional competencies on the internal and external markets in the global economy we have identified a set of elements that form the employee competitiveness, which we have structured in the following components:

– personal;
– professional.

On the first and second stages of determining the content of the elements, that form the employee competitiveness, a questionnaire to respondents is developed. It focuses on the characteristics that influence the results of professional activity, larger salaries, promotion, etc.

On the third stage the results are recorded in MS Excel to import them in STATISTICA6.

Marketing method – research is used to obtain quantitative data. The results are recorded in the form of answers – questionnaire.

Each item is scored on a 100 point scale, depending on the issue. Then the results are added to MS Excel database, summarized and recorded in STATISTICA 6 , which the data is processed with. The program will identify the characteristics that have the greatest influence on the formation and development of competitiveness.

The fourth stage is data processing. Processing of results is carried out using the principal components analysis used in Chemometrics for solving various tasks. This method is based on factor analysis and the construction of the correlation matrix.

The reliability of the data obtained can be checked using the Scree test, a graphical method first proposed by Cattell; factor loadings; the plotting scale.

The principal component analysis and STATISTICA 6 has allowed us to obtain representative data of 295 respondents. Nineteen principal components (elements) that have the greatest impact, determine the structure and form employee competitiveness has been selected.

1) education;
2) gender;
3) mental capacity;
4) speed of work;
5) tasks complexity;
6) the amount of work;
7) professional experience;
8) planning and organization;
9) decision-making;
10) coordination and control of activities;
11) analytical thinking;
12) the ability to transfer knowledge and skills, the ability to teach;
13) independent investment;
14) responsibility for work results;
15) innovative forms of training at the enterprise;
16) additional opportunities for health improvement, physical culture and sport for workers and family members; cultural and leisure activities;
17) corporate pensions programs;
18) personnel reserve programs,
19) the development of corporate social programs.

The construction of mathematical model has identified gender as one of the elements of employee competitiveness formation. The issue of gender segregation in labour market was raised long ago, but it’s hard to determine who is the most competitive. This question deserves separate scientific research.

The data obtained in the result of mathematical analysis allow to note that the selected dominant elements are part of employee competitiveness and directly involved in its formation.

The elements that form the competitiveness are marked as dominant, because we cannot accurately determine the baseline composition of the elements of employee competiveness. In a constantly changing situation and taking into account different levels (national, regional, and of an enterprise) some of the elements will have a greater impact, others will have less impact on employment and wages in a particular region, an enterprise. For example, employees competitiveness in Lipetsk region may be lower than the competitiveness of Voronezh region workers, and a Russian worker may be uncompetitive in comparison with the European one.

The presence of the dominant elements of competitiveness will allow employees to be more mobile on the territory of Russia and work in any region, but taking into account the prior training and adaptation in a specific industry. Therefore, the elements of competitiveness are dominant.

Before entering external labor market a worker needs to build competitiveness at the state level, and then to promote his or her level of competitiveness to the level of a particular country.

The fifth stage is to hold a point evaluation by experts (to determine the level of development of each element and the aggregate level). To determine the level of competitiveness on internal or external labor markets, an employee or an employer is recommended to focus on the given example of the matrix of employees competitiveness assessment in the conditions of economic globalization, which was tested at the enterprises in Lipetsk and Moscow regions. A fragment of matrix is shown in Table 1.

Table 1.

A fragment of matrix of employees competitiveness assessment

Full Name	Coefficients					∑points	Employee competitiveness level	Employee appraiser recommendations
	1	2	…	16	17			
Malinin I.V.	100	100	…	100	100	1700	high	to maintain the level, intangible motivation

Each indicator has a maximum of 100 points, thus, when all indicators are added, the maximum sum that determines employees competitiveness is 1900 points. If you do not consider the gender indicator, the maximum is 1800 points.

Taking into account changes in the number of coefficients the amount is 1700 or 1600 as a result of additional mathematical analysis, and the level of employees competitiveness is determined by comparison in the organization, then the amount may be:

1700/1600 − 1320 − high level;

1319 − 939 − upper – intermediate level;

938 − 558 − intermediate level;

557 − 177 − pre – intermediate level;

176 − 0 − low level.

The competitiveness level is determined from the received amount of points. Further recommendations to improve the situation or solve the problem are given. It depends on the coefficient with the least points.

The sixth stage is represented, in this case, in the form of indicators adjustments and allocation formulas. The number of indicators has become less and the dominant elements are 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17.

It should also be pointed out that a specific structure of dominant elements of competitiveness allows taking into account the impact of the environment. Thus, the degree of negative influence of economic globalization technological factors allows to reduce the impact of the environment and use the opportunity of C1, C3, C7, C15; regulatory factor C13, C14, C16, C17; factor of production C4, C5; infrastructure condition factor C6, C8, C9, C10, C11. However, the distribution of elements is not static, so the content of each element may vary depending on the level that forms it.

Since the assessment of indexes throughout the entire process of formation and development is changing, for each of them we have assigned constant weighting factor.

To get more accurate data, weighting factors which correspond to employees competitiveness assessment indexes have been determined (formula 1).

Quantitative value of weighting factor was assigned by determining the proportionality of index value and total variance. The formula is represented as:

$$CPT_{emp} = 0{,}07 \times C_1 + 0{,}07 \times C_2 + 0{,}07 \times C_3 + 0{,}06 \times C_4 + 0{,}07 \times \\ \times C_5 + 0{,}07 \times C_6 + 0{,}08 \times C_7 + 0{,}07 \times C_8 + 0{,}07 \times C_9 + 0{,}07 \times C_{10} + \\ + 0{,}07 \times C_{11} + 0{,}06 \times C_{12} + 0{,}07 \times C_{13} + 0{,}06 \times C_{14} + 0{,}10 \times C_{15} + \\ + 0{,}09 \times C_{16} + 0{,}09 \times C_{17}. \quad (1)$$

The final stage of the assessment in the given method is to rank and determine the total level of the development of the elements, which form employees competitiveness. This is quantitative assessment of the level of employees competitiveness (tab. 2).

Table 2.

Example of calculating the employee competitiveness level

Full name	Employee competitiveness calculation	Employee competitiveness level, %
Malinin I.V.	0,07×100+0,07×100+0,07×100+0,06×100+0,07×100 +0,07×100+0,08×100+,07×100+0,07×100+0,07×100 +0,07×100+0,06×100+0,07×100+0,06×100+0,10×10 0+0,09×100+0,09×100=115	115/100 = 1,15

The ranking is done according to the following rank:

$C_{cpt} \geq 1$ – high level of competitiveness;

$0{,}75 \leq C_{cpt} < 1$ – upper-intermediate level;

$0{,}5 \leq C_{cpt} < 0{,}75$ – intermediate level;

$0{,}25 \leq C_{cpt} < 0{,}5$ – pre-intermediate level;

$0 \leq C_{cpt} < 0{,}25$ – low level.

Conclusion

The proposed method allows:

– to assess the level of employee competitiveness taking into account the requirements which are formed under economic globalization and are imposed to the quality of workforce, professional competencies on external and internal markets;
– to identify items that do not match the criterion level;
– to make recommendations to form or develop the dominant elements of competitiveness considering the environment challenges and the strategic objectives of a company, region, country;
– to form the basis to improve motivation policies at all levels.

It's necessary to note that there are some errors, which depend on industry-specific post and its requirements; the employee location (internal or external labour market), etc. Structure and content of the elements that form the employee competitiveness may vary.

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ANALYTICAL SYNTHESIS OF CHEMICAL REACTOR CONTROL SYSTEM

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The problem of the analytical synthesis of the synergetic control system of chemical reactor for the realization of a complex series-parallel exothermal reaction has been solved. The synthesis of control principles is performed using the analytical design method of aggregated regulators. Synthesized nonlinear control system solves the problem of stabilization of the concentration of target component at the exit of reactor and also enables one to automatically transfer to new production using the equipment.

Keywords: *analytical synthesis; control system; chemical reactor; synergetic control theory; computer simulation.*

Introduction

The fundamental concept of the design of contemporary flow processes is the concept of the design of cybernetically organized chemical engineering processes and systems, which was rationalized by Academician V.V. Kafarov [1].

According to this concept, during the step of the design of chemical production, which is related to the conversion of initial substances to final products, the problem of optimal synthesis of reactor junction and problem of synthesis of the process control algorithms is solved; and, at the step of consumption, the sub-problem of the organization of optimal functioning of object under the effect of parametrical and signal disturbances [1–5].

Despite the large number of the works related to the automation and control of chemical reactors [6–9], the problem of synthesizing control systems that provide the maintenance of optimal modes of their work remains completely unsolved. This is related to the principal feature of chemical reactors as control objects, namely, manifold, nonlinearity, and multicoupling.

The solution of this situation is to develop a physical theory of control, in particular synergetic control theory, the principal features of which were formulated in [10–12].

The use of synergism ideas in the problems of control assumes the development and realization of the directed target self-organization of object-regulator dissipative nonlinear systems. Furthermore, the aim of the motion of system is formulated as the desired invariant manifold in phase space of object, which acts as a target attractor [12].

In general, the problem of synergetic synthesis of the control system is formulated as follows: the control principle, $u = (u_1,..., u_m)^T$, should be determined as the function of state variables of object $u_1(x_1,..., x_n)$, ..., $u_m(x_1,..., x_n)$, which transforms the representative point (RP) of system in phase space from the random initial state to the environment of the given invariant manifolds $\Psi_S (x_1,..., x_n) = 0$, $S = 1,..., m$ and subsequent motion along the intersection of manifolds to somewhat stationary point or to somewhat dynamic mode. In the given equations, n is the dimensionality of state vector and m is the number of external controls. On the path of motion, the minimum of the criterion of optimality of system (J) should be attained and its stability should be ensured as follows:

$$\mathrm{J} = \int_0^\infty \left[\sum_{S=1}^{m} \left(T_S^2 \dot{\psi}_S^2 + \psi_S^2 \right) \right] d\tau. \qquad (1)$$

The motion of RP in phase space follows the functional equation

$$T_S \dot{\psi}_S + \psi_S = 0,\ S = 1,..., m, \qquad (2)$$

where T_S is time constant. This is the equation of stable critical point, which gives minimum to the optimizing functional (1). The condition of asymptotic stability of system generally has the form $T_S > 0$.

The effectiveness of the method of analytical design of control algorithms by nonlinear objects with the use of synergetic principle (the method of analytical design of aggregated regulators (ADAR)) is given in [13–16].

In this work, the problem of synthesizing the effective control algorithms of the chemical reactor in the realization of the complex series-parallel reaction is stated. The synthesized control system should provide the stabilization of the concentration of target component of chemical reaction on the exit of device under the action of disturbances on object, as well as the transfer of object from one mode of work to another (switch), namely, change of its productivity with the retention of the required quality of target component.

Description of object and statement of control problem

A chemical reactor is a capacity-type device equipped with a mechanical stirrer (Fig. 1). The device functions in isothermal mode. The multistep series-parallel reaction is carried out in the reactor as follows:

$$A + B \xrightarrow{k_1} P_1,\ A + P_1 \xrightarrow{k_2} P_2,\ A + P_2 \xrightarrow{k_3} P_3,$$

where A and B are initial reagents; P_1, P_2 and P_3 are products of reaction; k_1, k_2, and are rate constants of steps. The key component is P_2 substance. Initial reagents A and B are given to the device by separate flows.

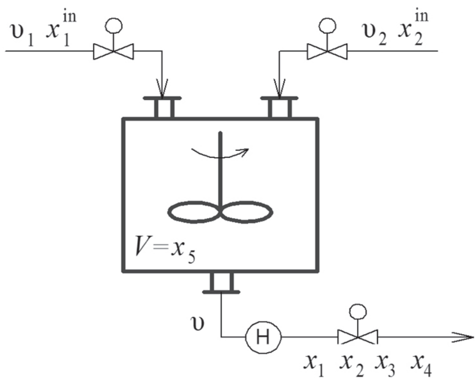

Fig. 1. Flow scheme of chemical reactor

In Fig. 1, the following designations are given: x_1^{in}, x_2^{in} are the concentrations of initial reagents; υ_1, υ_2 is the use of initial reagents; υ is the use of reaction mixture on the exit from device; x_1, x_2, x_3, and x_4 are the concentrations of components A, B, P_1, and P_2 in reactor; and $V = x_5$ is the volume of reaction mixture in device.

The mathematical model of chemical reactor at constant temperature of reaction mixture and variable degree (volume) has the following form:

$$\frac{dx_1}{d\tau} = R_1 + \frac{\upsilon_1 x_1^{\text{in}}}{x_5} - \frac{\upsilon x_1}{x_5}, \quad \frac{dx_2}{d\tau} = R_2 + \frac{\upsilon_2 x_2^{\text{in}}}{x_5} - \frac{\upsilon x_2}{x_5}, \quad \frac{dx_3}{d\tau} = R_3 - \frac{\upsilon x_3}{x_5},$$
$$\frac{dx_4}{d\tau} = R_4 - \frac{\upsilon x_4}{x_5}, \quad \frac{dx_5}{d\tau} = \upsilon_1 + \upsilon_2 - \upsilon, \qquad (3)$$

where $R_1 = -k_1x_1x_2 - k_2x_1x_3 - k_3x_1x_4$, $R_2 = -k_1x_1x_2$, $R_3 = k_1x_1x_2 - k_2x_1x_3$, $R_4 = k_2x_1x_3 - k_3x_1x_4$ is the rate of reaction on components.

The problem of control of chemical reactor is formulated as follows: one should synthesize the control principle, which provides the transfer of device from one production, $G = \bar{x}_4\upsilon$, to new production, $\bar{G} = \bar{x}_4\bar{\upsilon}$, and stabilization of the concentration of target component at the given degree $\bar{x}_4$ under the action of disturbances. The change of the output flow with time from υ to $\bar{\upsilon}$ can proceed by any principle, including in a stepwise manner.

The transfer to new production $\bar{G}$, with the maintenance of the given concentration $\bar{x}_4$, is made possible by the selection of the particular value of the average time of reaction mixture in device, $\bar{\tau}$. At the given $\bar{G}$, $\bar{x}_4$, $\bar{\upsilon}$, the required mean time can be achieved by the change in the mixture volume in the device.

The flow of the initial reagent υ_2 at the input to the device is suggested as the control effect for the volume regulation. In addition, one should also choose the control for stabilizing the concentration x_4 at the given degree under the action of disturbances. The analysis of the structure of equations of mathematical model of reactor (3) shows that variables x_1 and x_3 may act as the internal controls and the direct external effect can be performed only on x_1 by the change of the consumption of initial reagent υ_1 at the input to reactor. Thus, the control channels of the concentration of the target component and volume of the mixture in the device are represented as follows: $u_1 \to x_1 \to x_4$, $u_2 \to x_5$, where $u_1 = x_1$, $u_2 = x_2$.

Synthesis of control principles via ADAR

Because the mathematical model of object (3) contains two external controlling effects $u_1 = \upsilon_1$ and $u_2 = \upsilon_2$, we use the ADAR method on the basis of parallel-series combination of invariant manifolds [12]. The procedure for synthesizing the control principle involves the following. At the first step, the invariant manifolds are considered as shown below:

$$\psi_S(x_1, ..., x_5) = 0, S = 1, 2,$$

which determines the given relationships between phase coordinates of object, which in turn reflects the specificity of control object and requirements of designer to system. The control principle $u = (u_1, u_2)^T$ is synthesized so as to perform the transition of representative point of system in phase space from arbitrary initial position to the intersection of manifolds, $\psi_{1,2}(x_1, ..., x_5) = 0$.

Let us introduce two aggregated macrovariables to consideration, the first of which determines the relationship of x_1 with controlled variable x_4 and the second reflects the technological requirement to the volume of reaction system as follows:

$$\psi_1 = x_1 + \nu_1(x_4),\ \psi_2 = x_5 - \bar{x}_5, \tag{4}$$

where $\nu_1(x_4)$ is somewhat function, which should be determined at subsequent procedure of synthesis. Macrovariables (4) should follow the solution of principal functional equation of ADAR method (2).

Let us introduce the macrovariables Ψ_1 and Ψ_2 of Eq. (4) to functional equation (2) for the synthesis of control principle, $u = (u_1, u_2)^T$. As a result, we obtain the following equations:

$$T_1\left[\frac{\mathrm{d}x_1}{\mathrm{d}\tau}+\frac{\partial \nu_1}{\partial x_4}\frac{\mathrm{d}x_4}{\mathrm{d}\tau}\right]+x_1+\nu_1=0\ ,\ T_2\frac{\mathrm{d}x_5}{\mathrm{d}\tau}+x_5-\bar{x}_5=0\ .$$

Due to the equations of object (3), these relationships have the following form:

$$T_1\left[R_1+\frac{u_1x_1^{\mathrm{in}}}{x_5}-\frac{\bar{\upsilon}x_1}{x_5}+\frac{\partial \nu_1}{\partial x_4}\left(R_4-\frac{\bar{\upsilon}x_4}{x_5}\right)\right]+x_1+\nu_1=0, \qquad (5)$$
$$T_2(u_1+u_2-\bar{\upsilon})+x_5-\bar{x}_5=0,$$

where $\bar{\upsilon}$ is the new set value of the consumption at the exit from reactor, which determines the required production.

We obtain the following relationships for the control principle from Eq. (5):

$$u_1=-\frac{(x_1+\nu_1)x_5}{T_1x_1^{\mathrm{in}}}-\frac{R_1x_5}{x_1^{\mathrm{in}}}+\frac{\bar{\upsilon}x_1}{x_1^{\mathrm{in}}}-\frac{\partial \nu_1}{\partial x_4}\frac{(R_4x_5-x_4\bar{\upsilon})}{x_1^{\mathrm{in}}}, \qquad (6)$$
$$u_2=-\frac{(x_5-\bar{x}_5)}{T_2}+\bar{\upsilon}-u_1.$$

Controls u_1 and u_2 transfer the RP of the system in the phase space to the intersection of manifolds, $\Psi_1 = 0$ and $\Psi_2 = 0$, where the relationships $x_1 = -\nu_1$, $x_5 = \bar{x}_5$ are realized and the compression of phase space is realized, i.e., a decrease occurs in the dimensionality of the system of equations (3). The equations of decomposed system with the assumption of relationships $x_1 = -\nu_1$ and $\upsilon = \bar{\upsilon}$ have the following form:

$$\frac{\mathrm{d}x_2}{\mathrm{d}\tau}=R_2+\frac{u_2x_2^{\mathrm{in}}}{x_5}-\frac{\bar{\upsilon}x_2}{x_5},\ \frac{\mathrm{d}x_3}{\mathrm{d}\tau}=R_3-\frac{\bar{\upsilon}x_3}{x_5},\ \frac{\mathrm{d}x_4}{\mathrm{d}\tau}=R_4-\frac{\bar{\upsilon}x_4}{x_5}, \qquad (7)$$

where $R_2 = k_1\nu_1x_2$, $R_3 = -k_1\nu_1x_2 + k_2\nu_1x_3$, $R_4 = -k_2\nu_1x_3 + k_3\nu_1x_4$.

The function $\nu_1(x_4)$ in the decomposed system (7) can be considered to be the internal control, under the action of which the motion of object (7) along the intersection of manifolds $\Psi_{1,2} = 0$ takes place. At the second step of procedure, the investigation of the expression for $\nu_1(x_4)$ is performed. For this purpose, the aim of the motion of system

(7) is considered in the form of invariant manifold, which reflects the technological requirement to system as follows:

$$\Psi_3 = x_3 - \bar{x}_4 = 0. \tag{8}$$

Macrovariable Ψ_3 corresponds to the solution of functional equation, $T_3\dot{\psi}_3 + \psi_3 = 0$, which has the following form in extended form with the assumption of Eq. (8) due to the model of decomposed system (7) shown below:

$$T_3\left(-k_2\nu_1 x_3 + k_3\nu_1 x_4 - \frac{\bar{\upsilon}x_4}{x_5}\right) + x_4 - \bar{x}_4 = 0. \tag{9}$$

The internal control is written as follows in accordance with Eq. (9):

$$\nu_1 = \frac{x_4 - \bar{x}_4}{T_3(k_2x_3 - k_3x_4)} - \frac{x_4\bar{\upsilon}}{x_5(k_2x_3 - k_3x_4)}. \tag{10}$$

Final equation for the control principle u_1 can be obtained by the introduction of ν_1 function (10) and its partial derivative $\partial\nu_1 / \partial x_4$ to Eq. (6). The parameters of the adjustment of control laws, which affect the quality of the dynamics of the processes in object-regulator isolated system, are the time constants T_1, T_2 and T_3. The conditions of asymptotic stability have the following form: $T_1>0$, $T_2>0$, $T_3>0$.

Mathematical simulation and results

In order to verify the operation of the synthesized control law by the chemical reactor, the computer simulation of the object-regulator isolated system was performed. Properties of the control system, such as the ability (transfer) of the chemical reactor to switch from one mode of work to another (transfer to new production), disturbance invariance, covariance to the given actions, and the asymptotic stability of isolated system, were also studied.

The simulation was performed with the following technological and constructive parameters of object: $V = \bar{x}_5 = 500$ L, $x_1^{\text{in}} = 19.74$ mol/L, $x_2^{\text{in}} = 10.93$ mol/L, $\upsilon_1 = 1.5$ L/min, $\upsilon_2 = 3.5$ L/min, $\upsilon = 5$ L/min, activation energy $E_1 = 60300$ J/mol, preexponential multiplier of rate constant k_1 $k_{10} = 109860$ L/(mol min), ratios of rate constants of consecutive steps $k_2 k_1 = 2$, $k_3 k_1 = 2.5$, and the given concentration of target component $\bar{x}_4 = 0.54$ mol/L. The parameters of adjustment of regulators are $T_1 = 20$ min, $T_2 = 50$ min, and $T_3 = 50$ min.

In Figs. 2–4, the examples of transient control processes in the object-regulator isolated system are given with the transition from production $G = \bar{x}_4 \upsilon = 2.7$ mol/min to production $\overline{G} = \bar{x}_4 \bar{\upsilon} = 2.16$ mol/min by the change of stress. In Fig. 2, which demonstrates the change of regulated variables, the variant, when switching is performed in manual mode, is given.

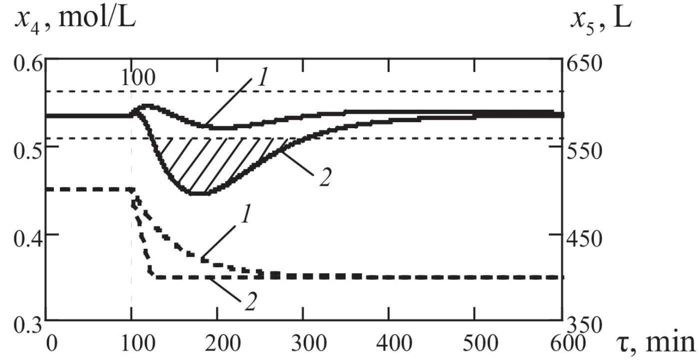

Fig. 2. Change of controlled variable x_4 (bold line) and the volume of mixture in device x_5 (dashed line) with decrease in load υ by 20%: (1) control system

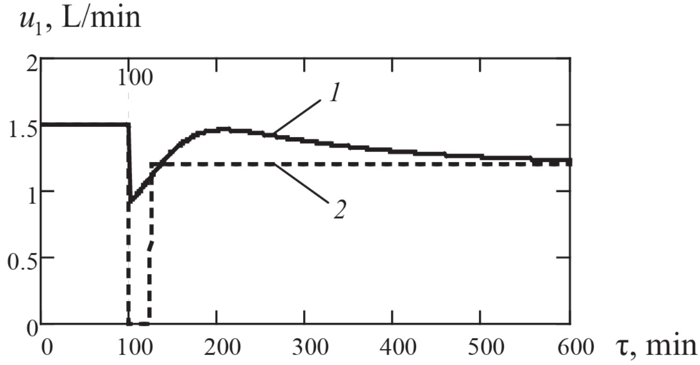

Fig. 3. Change in control action $u_1 = \upsilon_1$ with decrease in load υ by 20%: (1) control system and (2) manual mode

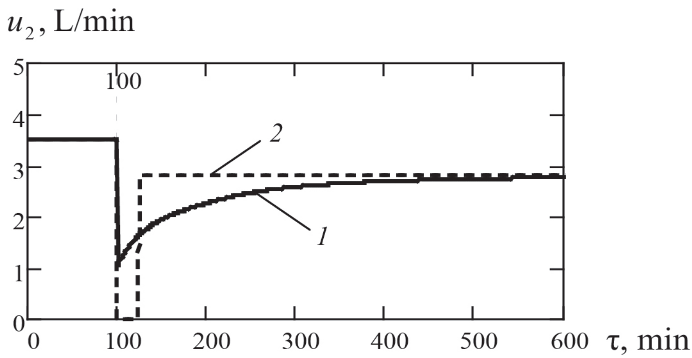

Fig. 4. Change in control action $u_2 = \upsilon_2$ with decrease in load υ by 20%: (1) control system and (2) manual mode

As follows from Fig. 2, the major drawback of the manual mode of transfer to new production is the large over-regulation on the concentration of target component, which leads to the loss of product.

Conclusions

In this work, the problem of the analytical synthesis of the control law of chemical reactor with the transition from one production to another was solved via the methods of synergetic theory. Computer simulation of the object-regulator isolated system confirmed these properties of synthesized control system as the ability to switch chemical reactor from one mode of work to another (transfer to new production), disturbance invariance, covariance to the given actions, and asymptotic stability. These facts make synergetic control theory very promising applied to such complex, manifold, and nonlinear objects of chemical engineering as chemical reactors.

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PROCESS APPROACH TO CULTURAL POLICY IN THE REGIONAL ASPECT

Lavryshsheva M., Kozlova L.

One of the most important social and political functions of any state is the cultural policy designed to regulate the inner life of civil society. Cultural factors are decisive in the creation of a harmonious society, but also in enhancing the intellectual and spiritual potential of the human capital which is the lead factor in the development of any state.

Characteristics of cultural policy, as a process, i.e. procedural approach, allows us to see the specific aspects of interaction of subjects over the governmental authorities. However, due to the fact, that in its scale cultural process is the same as political environment of the state, some scientists identify it either with politics in general or with the totality of the shares of behavioral government entities, change their status and influence. Supporters of the institutional approach associates the cultural political process with the functioning and the transformation of the government institutionы, based on a set of the political system reactions on the environmental challenges. As we speak in the current economic conditions in Ukraine is actual the development of anti-crisis measures for the rehabilitation and development of the conceptual approach of cultural policies in the region. As such, the obvious is the development of a measures set by all courses of the plan, that will mutualize the key goals, objectives and tools into a uniform system of measures. This plan should provide the combined model in the region and provide a transition to the zonal management principle of the transition period. In the plan it is also should be provided institutional support for the proposed measures, namely the mechanisms *of technological and socio-cultural issues implementation in range of the cultural policy of the society* [1, p.18].

Keywords: *cultural policy; political process; political actor; political institution.*

Introduction

Among culture and politics, there is no less close relationship than that between culture and economy. To grow and be passed from generation to generation, culture needs to be supported by the political authorities and the state. In turn, the political power is in need of the culture to be approved and supported. One can say that culture and politics are experiencing a mutual attraction and mutual need for each other. Politicians have the special interest in art, because it composes the core and the highest expression of culture.

The state is the main policy instrument and is the same to culture. It is the part of the cultural management system, and occupies in this system the highest level. The other main management levels are the regional and municipal. Modern form of state participation in culture is a cultural policy, which is the coordination and control of all cultural activities related to the maintenance and operation of historical and cultural heritage, ensuring equal access for all to culture, the support of art and all kinds of art, as well as, the cultural presence in other countries, and the influence on them. The state provides financial (budget), administrative, legal and moral support for all types of cultural activities. Cultural functions of the state are a logical response to natural, necessary and extremely important needs of people and society. Cultural activity is the content of cultural policy.

The problems of state cultural policy as a factor of the society reform under political process specifics were studying by Astafev O.N., Balakshin A.S., Vostryakov A.E., Drozhzhina S.V., Izhikova N.V., Karpuhin O.I., Malimon V.M., Michailovich V.A. and etc.

It should be noted that the above-mentioned authors have dealt with issues of cultural policy at the central level of the state. However, some issues are not covered in these studies, it wasn`t also sufficiently studied the special aspects of stabilization and implementation of cultural policies at local region in the transition level, the evaluation of political process applicability, the local transformations of political activity.

The political process structure

Some researchers consider the political process is a natural phenomenon that has an irrational character and dependent of the will and character of the people above all political leaders. The significance of random phenomena and events is particularly noticeable at the micro level. However, the general nature of politics and cultural policies as well as institutional and other contexts of the activity (rules, certain forms and modes of behavior, traditions and the dominant values, etc.) make the political process as normalized and comprehend. It is a logical unfolding sequence of interactions between people.

Thus, the political process is integral phenomenon amenable to structuring and scientific analysis. Unpredictability and seemingly inexplicable of certain events should be seen mainly as a consequence of the imperfection of scientific apparatus and tools [2, c. 45].

The political process structure can be described by the interaction analysis between the various political actors, as well as through the identification of dynamics (the main phases of the political process, the change of these phases, and so on) of this phenomenon. It is also important the factors clarification influenced the political process. Thus, the policy process structure can be defined as set of interactions between actors and their logical sequence (political process "plot"). Each individual policy process has its own structure and therefore their own "plot". Actors the totality of their interactions, sequence or the plot dynamics, the time units, as well as factors affecting the political process, usually are called the political process parameters, who are linked to the complexity of the concept of the process approach to the cultural policy of the society [3, p. 34].

The main factors of the political process are political systems, political institutions (government, civil society, political parties, etc.), organized and unorganized groups of people and individuals.

The Political institute is reproducible over time a set of rules and regulations, as well as institutional capacity, organize political relations in a particular area of political life [4, p. 62].

The main governance institution and one of the main political process actor is the state. Another important actor in the political process is civil society, which is also considered as a political institution. It should be noted that the state and civil society as political actors are generated in Europe and the US in new time period under the influence of modernization changes [5]. Since that time, it is formed the main government institution in society, which has a monopoly on coercive violence in a specific territory and it is named the state. At the same time, under the influence of this process it is formed the civil society, called the antithesis of the state. Civil society interacts with the state through cultural policies.

Smaller actors of the political process are the parties, interest groups, individuals and groups of people [6, p. 112].

Individuals and groups could engage in politics, not only in the institutional form, for example, vote in the elections, but also in the non-institutional forms, in the form of spontaneous mass protests.

People differ in varying degrees of activity in the cultural policy. The number of are not very active, but in general, are involved in most of the processes institutionalized. Some of just sit on the sidelines, not only by taking an active part in political life, but not participating in the elections, not reading newspapers, etc. Others of, however, this is usually a minority of citizens, on the other hand, take an active part in political life and to take into account the cultural policy society specificity as a whole.

To achieve group goals, individuals can create special groups, varying degrees of institutionalization of the random group formed at the meeting to a highly organized, which have the permanent character and valid according to the strict rules of the group's interests. The degree of political activities institutionalization depends not only the achievement of specific goals (as a rule, it is the more efficient than the higher the institutionalization degree), and reproducibility, repeatability, regularity of any political relations and their strengthening in the rules and regulations [7].

We will carry out a more detailed analysis of the political process from the point of view of regional development programs under the review of the cultural policy features.

In the analysis of the political process it should be taken into account the nature of the interaction between its subjects. It is important to note that the nature of the interaction depends on the scale of the political process and actors. In particular, the nature of the interaction between the political system and the environment will be determined by the level of the evolutionary development of the system and the environment, such as the degree of internal differentiation. At the same time, the nature of the interaction between actors, in particular between a citizen and a certain party, will be determined by other parameters: institutional conditions, the peculiarities of the party development, the party locate on the political system, the social and psychological characteristics of the individual, etc. In general, abstracting of the political processes and actors specifics, it is often described the nature of the interaction between actors in terms of confrontation, neutrality, compromise, union, consensus.

Two groups of factors of the political process can be identified: the "internal" and "external". By "external" refer environment (socio-economic, socio-cultural and other conditions) and its impact, the system, but "external" for the political process, political circumstances, such as the terms and conditions of the political game, "external" political events etc. By "internal" it may be include parameters such as the characteristics of the actors, their goals and intentions, the distribution of power resources, the logic and the "plot structure" of the political process [8].

An important parameter of the political process is its division into stages. Political processes of various kinds provide an example of a different stages combination. Diverse and uniformity of processes leads to the fact that highlight any steps that are common to all types of processes, is quite difficult. The various stages are the stages of the functioning of the political system, the electoral process or the process of creation and functioning of political parties. Therefore, the selection of specific steps appropriate in relation to certain types of political processes (Fig. 1).

The majority of the political actors interactions relate to the exercise of public power. For this reason, the process it is particularly great importance the adoption and implementation of political decisions. The analysis of this process is one of the most popular topics of foreign political science. Among researchers there is no consensus on the number and content of its stages.

Summarizing the different approaches, it can be associated with the following main phases:

– formulation of the problem (collecting the necessary information about the existing problems, public inquiries and possible solutions, the definition of primary and secondary problems);
– the formation of alternative solutions;
– comparative analysis and selection of the most effective solutions;
– the formation of public decision and its legitimation (through the adoption of laws, voting and so on.);
– implementation of the taken decisions;
– monitoring of the implementation and realization of "feedback".

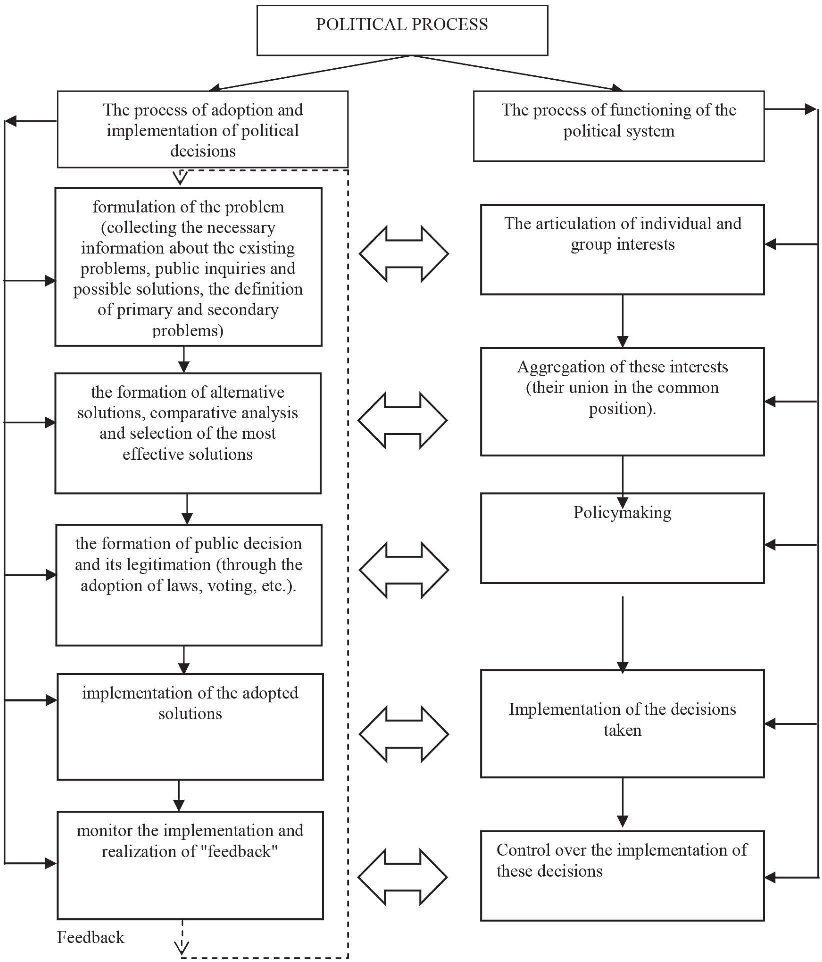

Fig. 1. Comparative characteristics of the political process

If we turn to the process of political system functioning, then a set of steps will be materially different, because it will take into account the interaction with the environment of the system. However, in science it is well known the attempts to highlight the main stages of this process it also focused on the adoption and implementation of management decisions. “A classic set “ of phase is to identify the main stages:

1. The articulation of individual and group interests.
2. Aggregation of these interests (their union in the common position).
3. Policymaking.
4. Implementation of the decisions taken.
5. Control over the execution of these decisions.

It should be noted that this model represents only one type of the political process and can not be regarded as universal.

Political changes and their types

Political changes are a specific type of social change related primarily to changes in the mechanism of regulation of the power of society. The political system under the influence of qualitative changes in the social environment is constantly in motion and development. In fact, there are not two identical states of the same political system. Consequently, political changes are transforming institutional structures, processes and goals that affect the distribution and administration of power management to developing society [9]. Political changes can occur either by adapting the system to the new requirements of the social environment, or by changing a system that is unable to maintain himself and the other. As part of the same society the political changes, that have a broad and lasting impact on society, can be described as a revolution. Revolution is a radical type of political changes, which resulted in the aborted old political tradition and the new political system of play.

Revolution as the type of policy changes should be distinguished from the insurrection. Last one is a sudden and unconstitutional change of the ruling elite, which is itself does not involve any profound changes in social relations. Revolutions and insurrections do not represent the most common type of political changes, though always cause permanent public interest [10, p. 89]. The most common type of change is a system adapting to new requirements or changes in the social environment. Such changes occur constantly in any well-functioning political system. They may be associated with the redistribution of political power under this society, with the introduction of constitutional changes in the power relations structure under the same political system, etc.

Conscious, systemic changes that have a broad and lasting impact on society, but reproduce the former political system, can be defined as reform. The reforms led to a change in the state of social and political relations under the existing political system. Therefore, the most important characteristic of the political process is the method or mode of political authority actualization (the reproduction of the political system).

The reform of political relations, changing the constitutional and legal methods and means of political authority realization under one political system and creates a certain political regime. Therefore, the concept of political regime characterizes the political process from the point of view of functioning and self-reproduction of a particular political system of this society.

Depending on the choice of fixed and variable characteristics of the political changes in the political science has developed two approaches: contextual and institutionalist. The first approach is based on the idea of the primary role of the social context, the social environment, socio-economic, socio-cultural conditioning of political and institutional change (Aron, R. Dahl, S. Lipset). The second approach focuses on the internal institutional structure of the political process. The nature and success of social change depends primarily on the level of political institutionalization. There are a variety of hesitation social environment, economic crises and public performances, but ultimately depends on the efficiency and adaptive response of institutional mechanisms to manage society, to maintain the stability of it (S. Huntington, T. Skolpol, D. March) [11, p. 43].

The variety of sources and forms of political change is expressed in certain ways to the existence of political phenomena, namely, the operation, development, and decline.

The functioning of political phenomena does not display relationships, behaviors of individuals or the execution of state power institutions of their direct functions beyond the established baseline values. For example, at the level of society as a whole is a way to maintain the current political system, the reproduction of the balance of power that reflects their basic relations, production of the main functions of structures and institutions, forms of cooperation between the elite and the electorate, political parties and local authorities, etc. In this way, changes in tradition and continuity have undisputed precedence over any innovations [12, p. 15].

The second method of political change is the development. He characterizes such modifications of basic parameters of political phenomena, which suggest further positive evolution of the latter. For example, in the scale of social development can mean such a change, in which the policy of the state is displayed on the level, which allows the authorities to respond adequately to the challenges of time, to manage public relations, to provide for the social demands of the population. This pattern of political change promotes compliance with the political system changes in other spheres of public life, improve its ability to use flexible strategies and technologies ruling based on the complexity of interests of different social groups and citizens [12, p. 16].

Finally, the third kind of change is a decline that characterizes such a process of transformation of the existing basic forms and relationships, which assumes a negative perspective of the evolution of political events. In the opinion of Struve, the decline is «regressive metamorphosis» policy. The decline political changes characterized by an increase in entropy, and the predominance of the centrifugal tendencies of integration. Therefore, the decline essentially means the collapse of the current political integrity (for example, the fall of the political regime, the dissolution of the party, state capture by external forces, etc.). In the scale of society such changes may indicate that the decisions regime less help him to effectively manage and regulate social relations, so that the regime loses its existence sufficient for the stability and legitimacy of the [12, p. 16].

Features of the political process

Coinciding in scale with the entire political space, a political process is not limited to conventional (contractual, regulatory) changes that characterize the behavioral actions, relationships and mechanisms of competition for state power, meeting the norms accepted in the society and the rules of the political game. Along with these political processes and capture the changes that reveal a violation of the subjects of their roles and functions set forth in the regulatory framework, abuse their powers, going beyond their political niche. Thus, the content of the political process in the fall and the changes that take place in the activity of subjects who do not share a common standard in the relationship with the government, for example, the activities of the parties in an irregular situation, terrorism, criminal acts of politicians in power, etc.

Reflecting really developed, not only the planned changes, the political process have a pronounced non-normative nature, which can be explained by the presence in the political space of various types of movement (wave, cyclic, linear, inversion, ie return, and others.) That have their own forms and methods of transformation of political phenomena, the combination of which deprives the latter of strict certainty and stability [2, p. 123].

From this perspective, the political process is a set of relatively independent, local transformations of the political activity of subjects (relationship, institutions) that occur at the intersection of a variety of factors and parameters which can not be accurately determined, and furthermore predicted. This political process is characterized by discrete changes or the ability to modify some parameters of the phenomenon and at the same time preserving intact his other traits and characteristics (for example, changing the composition of the government can be combined with the preservation of the old policy). The unique and discrete changes exclude the possibility of extrapolation (transferring values of modern facts for the future) of certain assessments of the political process, complicates political forecasting, foresight puts limits political prospects.

At the same time, each type of policy change has its own rhythmic (cyclical repetition), a combination of steps and interactions of subjects, organizations, institutions. For example, the electoral process is formed in connection with the election cycles, so the political activity of the population is developing in accordance with the phases of the nomination of candidates in the legislative or executive bodies, discussing their candidates, election and control over their activities. Own Rhythm political processes can define decisions of the ruling parties. In the same period the qualitative reformation of public relations decisive influence on the functioning of public institutions and ways of political participation of the population have no solution of higher authorities, and some political events that change the balance and the balance of political forces. Such a «ragged» rhythm can set the political process, military coups and international crises, natural disasters, etc.

Reflecting the real, practical changes in the prevailing political phenomena, political process necessarily includes in its content and the relevant technology and action procedure. In other words, the political process demonstrates the nature of the changes, which is associated with the activity of a specific subject, is used in a particular time and in a particular place for him habitual ways and means of action. Therefore, the use of different technologies, even solutions of the homogeneous problems requires different changes in character. Thus, without this level of technocratic policy changes become abstract, losing its specificity and concrete historical design.

The regional dimension of cultural policy.
In the works of Ukrainian researchers found several options to define the cultural policy.

In a broad sense, cultural policy is seen as a set of principles and standards, as well as a system of measures for the preservation, revitalization, development and expansion of the culture through a variety of state and public institutions. In a narrow sense, cultural policy – a state activity in the sphere of culture [13, p. 8].

Under the policy is a cultural activity of the representatives of various social circles, aimed at the formation of creative activity of the subject, the definition of the boundaries and conditions of work, selection, organization created cultural values, their coverage and consumption to achieve the objectives of the data subject, the most important of which are the reproduction of the existing system of social and political relations [14, p. 12].

Based on the above, the concept of cultural policies in the region (Donbass) can be defined as a set of anti-crisis measures at the national and regional level, aimed at regulating the activities of the subjects of the cultural life of the region, as well as processes that are aimed at the restoration and further development of the culture of the region during the transitional period.

It should be noted that cultural policy is a socio-cultural process governing relations between members of society, where regulators will act as norms of behavior.

State cultural policy must necessarily be paternalistic, but it can not be seen as charity, it is the duty of the state, it must focus not only on today's cultural needs of the population, but also take into account the long-term public interest in this area. Meritornaya State practice aimed at the formation and promotion of lagging demand "desired company", therefore, the concept of regulation of the population of consumer culture is well within the scope of the positional Enlightenment cultural policy and its objective: the creation of a field for a free and creative self-realization [15, p. 14].

Given the transition of Donbass and radical social transformation in this territory, the process of developing cultural policy is of paramount importance in the preparation of anti-crisis strategic plan for development of the region, since the quality of the cultural policy will depend on the ability of society and a measure of perception of political and administrative reforms and social transformations.

Implementation of modern cultural policy involves consideration of a number of principles, namely:

- Presence in the organization, which is involved in the political process, own position on the relationship of politics and culture;
- A permanent influence on the processes of relations with the state of politics and culture;
- Determination of priorities in the field of creativity and of the quality evaluation system of cultural products, which is a prerequisite for the implementation of cultural policies;
- An objective relationship between the degree of influence of the subject of cultural policy on the processes that occur in the field of culture and the amount of material resources attracted them;
- The dependence of the specifics of the implementation of the cultural policy of the social and political factors specific to the company [14, p. 13];
- Multiculturalism (processes, attitudes, politics and cultural diverse society based on freedom of expression, cultural experience, the definition of cultural diversity, cultural, ideological, political, religious pluralism, the definition of minority rights, both at the public and at the state level, tolerance);
- Cultural democracy;
- Attracting cultural identity in case of failure of the self-imposition;
- The preservation and development of linguistic diversity;
- Focus on the development of cultural policy creation;
- Focus both on national and universal values;

- Determination of the priority of international legal acts in the sphere of culture [16, p. 15].

If we talk about the Donbass during the transitional period, this list may be supplemented by the following principle of modern cultural policy:

- The unity of the information field in the region, which has a dramatic impact on the formation of the main directions of the cultural policy of the territory;
- Unity and integrity of the cultural space in the region;
- The personification of the cultural policy, that is, identifying the link between cultural processes and their developers.

Most scientists agree on the general opinion that cultural policy is one of the most important components of the sustainable development of a given territory, which is controlled by society as a whole and the State in particular.

Support and regulation of culture carries primarily society through local governments, private investment, donations, sponsorship, as well as the state itself through the redistribution of budget revenues, grants, investments at low interest rates, targeted funding, legal framework, counseling, information support.

Regional culture should be supported by resource capabilities, namely the formation of territorial (regional) cultural development fund. The region should be the main level at which the regulation of cultural life.

The strategically important area of cultural policy should be Donbass protectionism and promoting cultural region of the platform, which will be based on an understanding of its weighty significance in the world, value and spiritual development of the individual.

The basis for the creation of a new system of legal regulation of the region's cultural policy should be a legal basis which will regulate philanthropy. Cultural policy Donbass needs to create a legal framework to promote initiatives in the field of philanthropy and supporting these initiatives.

It should be understood that for a qualitative and efficient carrying out of cultural policies in the region of one of the state support is not enough. The state, in turn, creates only the external conditions for the cultural development. In this case, we have the following relationship: "the state – region – personality." That is, the state should create conditions for a cultural policy in the region, the region should provide opportunities for cultural development of the region's inhabitants, and every person is a carrier of the traditions of the region, and, therefore, is the basis for self-culture.

The cultural heritage of the Donbass is one of the forms of collective memory. Being in the zone of conflict, there is a risk of destruction of the unique resources of the region. Therefore, the cultural heritage of today requires special protection and attention. In this regard, it considered appropriate:

- To improve the mechanism of protection and conservation of the region's cultural heritage by: legal protection; financial and resource support of cultural institutions; development and implementation of comprehensive security plan and the preservation of cultural heritage; enhancing international cooperation in the field of cultural policy.

All of the above should be reflected in the development of the mechanism of protection of the cultural heritage of the region.

Detachment of the state of ill effects on the cultural sphere as well as the independence of the cultural institutions, their funding, and preferential tax support, financial and legal independence of the region – is the necessary steps for the improvement of cultural policies in the region.

Conclusions

Thus, the term "cultural policy" is one of those meaningful control which illustrates the nature of the cultural and civilizational processes in Ukraine. The official discourse of this phrase includes the variability of its realization. In particular, given the infrastructural and operational level to ensure the cultural policy in Ukraine, it can be perceived as a ritual formula, in the Soviet period had a certain ideological burden, and now – only symbolically reproduces the image of the state in the process of modeling a certain value paradigm. Given its scientific and theoretical support in existing concepts and programs have reason to conclude that the declaration of the state cultural policy intentions to modernize the system of spiritual values of society. And in fact, and in another case, the problem remains a degree of coincidence of culture content in projects of power and the practice of social activities. In fact, this is an attempt to combine the two strategies in a single formula. The choice in favor of modernization or kulturohranitelskimi draft cultural policy of the state can be caused as a strategic goal, and the presence of a specific mechanism for their implementation.

Therefore, the priority task of the region's cultural policy should be to create a new cultural infrastructure that will meet the requirements of the market economy, democracy and civil society. To do this: create an adequate existing legal framework of the cultural policy in the transitional development of the region; create non-state institutions of culture; to provide at the national level for the protection of cultural products through targeted taxation of its producers. These steps will contribute to the development of cultural industries in the region. Enhancing the region's cultural policy will not only have a positive socio-economic impact on the state as a whole, but also will contribute to the consolidation of civil society in the country.

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CONCERNING CHAIN GROWTH SPECIFIC REACTION RATE AS A PART OF THE PROCESS OF METHYL METHACRYLATE MASS RADICAL POLYMERIZATION

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It is the chain growth specific reaction rate that was determined for the process of methyl methacrylate mass radical polymerization within the temperature range of 40–900 C in quasi-steady approximation by means of Monte Carlo method. The theoretical model of radical polymerization was developed taking the gel effect into account. Computer software was developed that enables to imitate radical polymerization process taking gel effect into account within the minimum run time. The programme was tested on asymptotic examples as well as was applied for methyl methacrylate mass radical polymerization. The programme makes it possible to calculate monomer conversion, molecular mass variation, molecular-mass distribution, etc.

Keywords: *chain growth specific reaction rate; gel effect; methyl methacrylate; Monte Carlo method; mass radical polymerization.*

Introduction

Radical polymerization process has been of great interest not only due to its significant practical value and the need to improve ways to control this complicated process, but also due to the rapid research development of the process's promising variants, namely, 'pseudolive', complex-radical, as well as radical-coordination polymerization variant. That, along with the improvement of experimental methods of research, contributes to developing methods of mathematical simulation of polymerization processes. The use of modern computing technologies ensures effective forecasting of kinetic regularities of polymerization, molecular structure and molecular mass characteristics of the products, as well as forecasting of practically relevant physical and chemical properties of polymers [1–4]. The application of computational methods is especially significant for the analysis of complex mechanisms of radical polymerization. The application of methods of mathematical simulation to the research of other types of catalytic polymerization [2–3], being unconditionally positive, proves this approach in the case of dealing with radical processes to be promising. However, it is even simulation of the standard mass radical polymerization of typical monomers that is not a trivial task. At the end of the 40s it was found that mass radical polymerization of methyl methacrylate (MMA) is accompanied by the gel effect [5], that is, a sharp increase in both the polymerization rate and molecular mass (MM) at considerably high conversions. Thus, while the MMA polymerization is taking place, acceleration can be observed at the conversion rate of 0.15–0.2 [6] or 0.6 [7]. Therefore, the gel effects should be taken into account while studying kinetics and determining the polymerization rate.

One of the models of taking the gel effect into account in the case of styrene polymerization is thought to be the Hui-Hamielec model. The model is based on empirical dependence of the chain termination reaction rate (k_t) on monomer conversion (x): $k_t = k_{t0}\cdot\exp(-E/RT)\cdot\exp(-2(A_1x + A_2x^2 + A_3x^3))$, where $k_{t0}\cdot\exp(-E/RT)$ is the chain termination reaction rate without taking the gel effect into account [8].

For the purposes of numerical simulation of MMA polymerization and quantitative correlation between the estimated and observed dependences one should know the exact real chain growth reaction rate (k_p) at various temperatures.

There are quite a lot of methods available for determining the value of k_p. In [9], chain growth reaction rate was found by interpreting the experimental data obtained by various researchers (Table 1). However, in general, the researchers determine the chain growth reaction rate value by interpreting their own experimental data only.

Table 1.

Chain growth reaction rate in the Arrhenius equation form $k_p = k_{p0} \cdot \exp(-E/RT)$

$k_{p0} \cdot 10^5$, L/(mol·sec)	E/R, K	Determination method	Ref.
6.6	2367	Interpretation of the experimental data	[9]
4.92	2198	SIP	[10]
4.9	2190	SIP	[11]
25	2766±300	Electron spin resonance	[12]

Until recently the main method of determining the chain growth reaction rate was thought to be the ‘rotating sector’ method [13]. The article [14] describes surface initiated polymerization (SIP). The SIP method is similar to the ‘rotating sector’ method as the monomer and initiator solution flows through an unlit tubular reactor past regularly placed splits that permit light through. The chain growth reaction rate determined using the SIP method can be found in [10–11] (Table 1). The value obtained was applied in [15–16] to describe mass radical polymerization of methyl methacrylate (MMA) in theory.

The ‘spin trapping’ method has become quite widespread for the purposes of obtaining data on the chain growth reaction rate. The method is based on the reaction of the non-paramagnetic molecule (trap) with a short-lived radical specifically placed into the medium under study, the result being formation of a stable radical that is characterized by having specific electron paramagnetic resonance. The use of spin trapping enables to identify short-lived radical products [17]. The chain growth reaction rate determined using the above-mentioned method can be found in [12] (Table 1).

The most reliable method of determining the chain growth reaction rate is thought to be pulsed-laser polymerization (PLP) [18]. The method consists in irradiating the vessel containing the monomer with high power pulsed laser radiation, which results in generating a considerable amount of radicals that destroy virtually all previously formed ones. The new radicals that survived initiate polymerization of new macroradicals that grow until the next pulse [19]. The value of k_p, relevant for MMA polymerization, was published in [19].

The study is aimed at determining the chain growth reaction rate in quasi-steady approximation as well as at simulating MMA mass polymerization using the Monte Carlo (MC) method taking the gel effect into account.

Model core

The following reactions were considered while simulating MMS polymerization:

substance initiation	$I \xrightarrow{k_d} 2R_0^{\bullet}$
chain growth	$R_p^{\bullet} + M \xrightarrow{k_p} R_{p+1}^{\bullet}$
chain transfer to monomer	$R_p^{\bullet} + M \xrightarrow{k_m} R_1^{\bullet} + P_p$
recombination	$R_p^{\bullet} + R_j^{\bullet} \xrightarrow{k_{com}} P_{p+j}$
disproportioning	$R_p^{\bullet} + R_j^{\bullet} \xrightarrow{k_{disp}} P_p + P_j$,

where I, M, $R^{\bullet}$, P are initiator, monomer, growing radical, 'dead' macromolecule; whereas index is the polymerization degree, k_d, k_p, k_m, k_{disp}, k_{com} are rates of substance initiation reaction, chain growth, chain transfer to monomer, disproportioning and macroradicals recombination.

A possible thermal initiation reaction was thought to be irrelevant due to the fact that PMMA synthesis simulation was carried out at relatively low temperatures. Also, chain transfer to initiator and polymer reactions were thought to be irrelevant due to their improbable nature.

The MMA polymerization process under study correlates to a system of differential equations:

$$\frac{d[I]}{dt} = -k_d \cdot [I] \quad (1)$$

$$\frac{d[M]}{dt} = -[R^\bullet]\cdot[M]\cdot(k_p + k_m) \qquad (2)$$

$$\frac{d[R^\bullet]}{dt} = 2\cdot f\cdot k_d\cdot[I] - [R^\bullet]^2\cdot(k_{disp} + k_{com}), \qquad (3)$$

where *f* is substance initiation reaction efficiency.

The simulation of MMA radical polymerization by azobisisobutyronitrile (AIBN) and benzoyl peroxide (PBO) involved reported values of reaction rates (Table 2).

Table 2.

Parameters values for simulation of MMA mass radical polymerization

Parameters	Values	Ref.
$k_{t0} = k_{rec} + k_{disp}$	$9.8\cdot10^7\cdot\exp(-353/T)$, L/(mol·sec)	[10]
k_t	$k_{t0}\cdot\exp(-2(A_1x+A_2x^2+A_3x^3))$	[8]
$n = k_{rec}/k_{disp}$	$3.956\cdot10^{-4}\cdot\exp(-2065/T)$	[20]
k_{disp}	$k_t\cdot n/(n+1)$, L/(mol·sec)	[21]
k_{com}	$k_t/(n+1)$, L/(mol·sec)	
f (AIBN)	0.5	[22]
k_d (AIBN)	$1.053\cdot10^{15}\cdot\exp(-15440/T)$, c^{-1}	
f (PBO)	1	[9]
k_d (PBO)	$1.18\cdot10^{14}\cdot\exp(-15097/T)$, c^{-1}	

Experimental part

MMA (by Fluka) was double distilled under vacuum. For the purposes of polymerization, the MMA fraction with $T_{boil} = 39^oC$ at $p = 100$ mmHG, $n_D^{20} = 1.4130$, $d_4^{20} = 0.936$ g/ml was used. The clarity degree of monomers was controlled using the method of MNR ^{1}H- and ^{13}C.

The AIBN and PBO initiators were double recrystallized from methanol and then were dried under vacuum at room temperature until the fixed mass value was reached.

Conversion dependences were obtained using the dilatometric method [6].

For the MMA mass polymerization the reaction mixture was poured into an ampule, then the solution was degassed by a triple cycle of freezing – defrosting till the residual pressure of 1.3 Pa was detected. The ampule was then sealed and placed in a thermostat (capable of maintaining ±0.1°C temperature accuracy) and kept until the required conversion degree was obtained, the one calculated using the formula:

$$x=DV/(V_0\times k),$$

where V_0 – monomer initial volume, DV – its variation, $k=(V_м-V_п)/V_м$ – contraction coefficient, $V_м$ и $V_п$ – monomer and polymer specific volumes [23]. Once polymerization had taken place, the ampules were cooled and opened. The polymeric product obtained was dissolved in acetone and then deposited with 10–15-fold excess of ethanol. The polymer was cleared of the rest of the initiator using triple redeposition. The polymer was then dried under vacuum (T=40°C) until the fixed mass value was reached.

Polymer molecular-mass distribution (MMD) and average molecular mass (MM) were determined by gel-permeation chromatography. The analyses were performed using a Waters GPC 2000 System liquid chromatograph (eluent: chloroform, flow speed: 0.5 ml/min). The pin system was calibrated according to polystyrene standards $\overline{M}_w / \overline{M}_n \leq 1.2$.

Determination of chain growth reaction rate in quasi-steady approximation

From the historical point of view, it is the method based on quasi-steady approximation that is the first to be used to determine the chain growth reaction rate. It was suggested that the chain termination rate fails to depend on conversion: $k_t=k_{t0}=const.$ Using $d[R^\cdot]/dt=0$ approximation, the quasi-steady macroradical concentration was calculated:

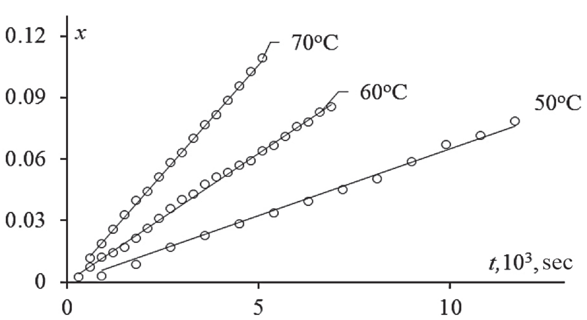
$$[R^\bullet]\approx\sqrt{\frac{2\cdot f\cdot k_d}{k_{t0}}[I]_0} \qquad (4)$$

as well as chain growth reaction rate was determined taking the initial polymerization rate into account:

$$k_p \approx \frac{V_{нач}}{[M]_0 \cdot [R^\bullet]} \quad (5)$$

where $[M]_0$=9.39 mol/L – initial monomer concentration.

The initial polymerization rate was determined by approximation of experimental conversion dependencies of the study as well as the data published in [24–29] using the least-square method on the initial section of the curve $x \le 0.15$ (Table 3). The initial section of conversion curves is approximated by linear dependence with a high correlation coefficient $r \ge 0.9964$ (Pic. 1).



Pic. 1. Typical initial section of MMA conversion, $[AIBN]_0$=1 mmol/L

Table 3.

Kinetic parameters of MMA mass polymerization

T, °C	Initiator	$[I]_0$, mmol/L	Ref.	$V_0 \cdot 10^5$, mol/(L·sec)			$[R^\bullet] \cdot 10^8$, mol/L	k_p, L/(mol·sec)
45	AIBN	6.25	[24]	5.90	±	0.20	1.3	480
	AIBN	12.5		10.0	±	1.0	1.9	560
	AIBN	25		12.5	±	8.7	2.6	509
	AIBN	50		16.7	±	1.4	3.7	480
	AIBN	100		22.0	±	5.0	5.2	427
	AIBN	200		29.52	±	0.15	7.4	425
								480±51**

End of Table 1.

	AIBN	1	*	4.11	±	0.02	0.8	580
	AIBN	3	*	7.3	±	0.08	1.3	595
	AIBN	15.48	[25]	14.2	±	3.7	3	485
50	AIBN	15.5	[25]	15.1	±	2.9	4.3	354
	AIBN	25.8	[26]	18.8	±	3.6	3	674
	AIBN	25.8	[26]	18.19	±	0.93	3.8	506
	PBO	43	[27]	15.73	±	0.31	4	421
								516±111**
	AIBN	1	*	11.38	±	0.04	1.5	797
	AIBN	3	*	19.57	±	0.19	2.9	708
	AIBN	5.6	[28]	22.5	±	1.0	3.6	688
	AIBN	11.2	[28]	30.5	±	0.66	5.1	617
60	AIBN	28	[28]	46.38	±	0.41	8	659
	AIBN	56	[28]	63.04	±	0.99	11.4	590
	AIBN	100	[29]	83.7	±	1.8	15.2	586
	PBO	1	*	8.610	±	0.01	1.2	761
	PBO	21.4	[27]	26.86	±	0.29	5.6	513
								658±78**
	AIBN	1	*	20.43	±	0.08	2.3	740
	AIBN	3	*	40.4	±	1.2	5.1	844
	AIBN	15.48	[25]	94.9	±	1.8	11.6	874
70	AIBN	15.5	[26]	86	±	37	11.6	794
	AIBN	25.8	[25]	110	±	16	15	788
	AIBN	25.8	[26]	119.8	±	7.1	14.9	854
	PBO	1	*	17.81	±	0.07	2.3	827
								817±46**
80	AIBN	3	*	85.89	±	0.17	9.5	964
	PBO	1	*	37.81	±	0.17	4.2	955
								959±6**
	AIBN	15.5	[26]	445	±	47	38.9	1220
90	AIBN	15.48	[25]	391	±	37	38.9	1071
	AIBN	25.8	[25]	460	±	181	50.1	978
								1146±122**

* – according to the study, ** – average values

k_p is determined with a considerable measurement uncertainty that is made by both statistical uncertainty, while determining the initial rate, and systematic uncertainty as a result of quasi-steady approximation applied. The former can be calculated precisely as the experimental data approximation takes place, the average relative uncertainty being 15%, that can correlate with the average statistical uncertainty while determining k_p according to the experimental data obtained by various researchers, i.e., 8% (Table 1).

The latter was determined as follows by differentiating the expressions (4–5):

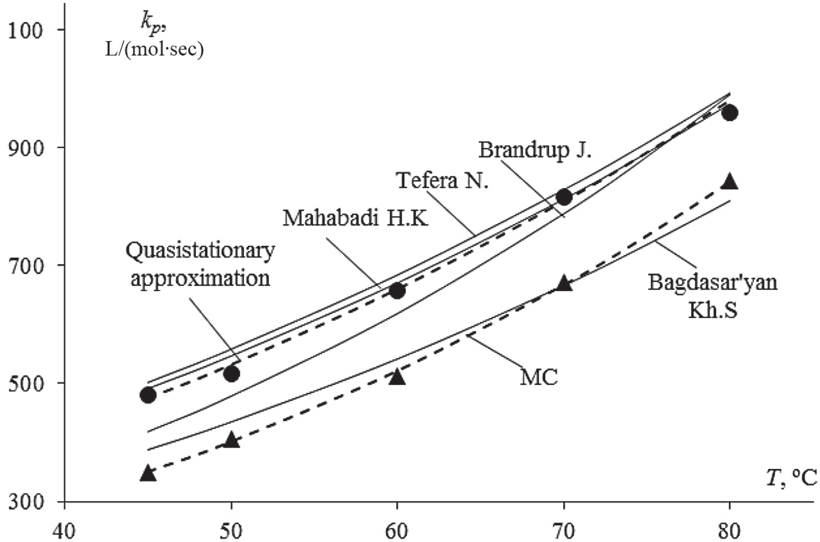
$$\frac{\Delta k_p}{k_p} = \frac{\Delta V}{V} + \frac{\Delta[R^\bullet]}{[R^\bullet]} + \frac{\Delta[M]_0}{[M]_0}, \quad \frac{\Delta[R^\bullet]}{[R^\bullet]} = \frac{1}{2}\left(\frac{\Delta[I]_0}{[I]_0} + \frac{\Delta k_{t_0}}{k_{t_0}}\right),$$

where $\Delta V/V$ is statistical uncertainty. Thus, monomer and initiator systematic uncertainty can be determined. In case the formulas (4–5) are used, then monomer concentration is thought to be intact. In fact, within the section 0–20% of the curve the concentration drops by 20%. The medial value $\Delta\ [M]_0/[M]_0$=10% was considered to be the uncertainty. Likewise, the initiator concentration is varied within the section to the value of $\Delta\ [I]_0/[I]_0$=10%. (AIBN, 60°C). In case these uncertainties fail to be taken into account, then the macroradicals concentration increases and there is a decrease in the value of the chain growth reaction rate.

The uncertainty, being the result of reducing the PMMA chain termination rate was determined using the Hui-Hamielec model [8]. According to the expression (5) the chain termination rate within the section 0–20% is reduced by 71% (60°C). This type of uncertainty results in k_p increase in quasi-steady approximation and partially compensates the uncertainties in the monomer and initiator concentrations.

Thus, it can be assumed that the systematic uncertainty, in case quasi-steady approximation is applied for the purposes of MMA polymerization, results in increasing k_p by 50%.

Having approximated the average values of chain growth reaction rates (Table 3) using the Arrhenius equation form, we obtained the following k_p value: k_p=7.26·10^5·exp(–2333/T). The value correlates with the ones published earlier that were determined using the SIP method [10–11] (Pic. 2).



Pic. 2. Temperature dependence of chain growth reaction rate by MMA polymerization

The chain growth reaction rates determined using the SIP method [10–11] were found on the initial polymerization section that proves the correct nature of the chain growth reaction rate value in quasi-steady approximation.

MMA polymerization simulation using the MC method Algorithm description

The MC method is thought to be an efficient for solving complex systems of equations. The classic algorithm of the MC method is to select events for each element of the assembly, using a pseudorandom number generator. However, there are cases when nothing happens to the selected element, and as time spent on the calculation depends on the number of the sensor's hit count, then the use of this approach considerably increases the amount of time spent on the calculation.

The proposed simulation algorithm, that uses the MC method, rules out non-productive hits that, in turn, increases the algorithm's efficiency.

It was assumed that at the initial time (t=0) the size of the assembly is equal to the initial number of initiator molecules. The entire polymerization process is divided into small time intervals (dt). The idea of the algorithm is that at each time step an assembly element number is randomly selected for the event. And for each element the event occurs with probability equal to unity. The number of random selections of acts at a step corresponds to the reaction rates. This simulation approach enables either to reduce the computer calculation time to a great extent or increase the statistical assembly [30, 31].

A single act of chain growth reaction occurs by increasing the number of main-chain links per unit. The number of monomer molecules is reduced by unity.

An act of chain transfer to monomer was simulated as follows. The assembly element number (macroradical) was selected, the one that contains a growing chain undergoing chain transfer reaction to monomer. At the time of the transfer, a 'dead' macromolecule is formed, its polymerization degree at the time of transfer being equal to the length of the growing molecule. At the time of the transfer, a new growing chain is formed, its length being equal to unity.

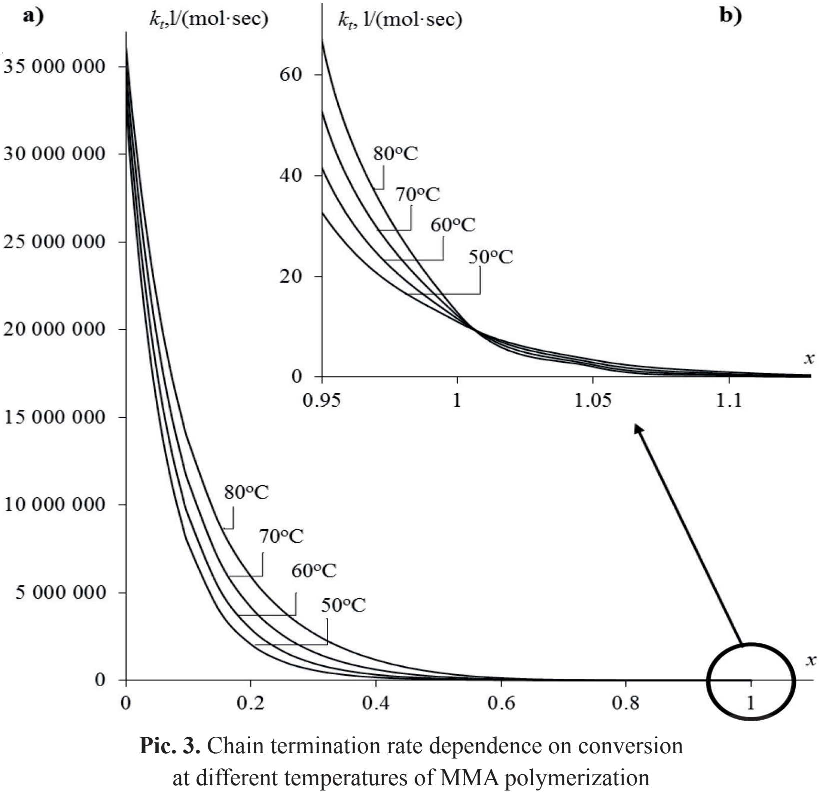
An act of chain termination is performed by one of two possible mechanisms: disproportioning or recombination. The number of two macroradicals was selected randomly at the time of one of the two possible chain termination reactions. When the macroradicals disproportioning takes place, two 'dead' macromolecules are formed with the correspondent chain lengths. When the recombination reaction takes place, one 'dead' macromolecule is formed with the chain length equal to the sum of the chain lengths of the collided radicals. The number of macroradicals as a result of the chain termination act was reduced by two unities.

When the simulation process took place, the number of 'dead' macromolecules with a specific chain length was counted, the ones being formed during the acts of chain transfer to monomer and chain termination; which allowed to determine the number-average and mass-average MM PMMA as well as molecular-mass distribution (MMD) at different polymerization periods.

The program was implemented in the Borland Delphi 7 software development kit, the calculations were made on the AMD Athlon PC (2.81 GHz, 2 GB). The run time is directly proportional to the size of the assembly, whereas it is the assembly size of 50–100 million initiator molecules that is thought to be quite sufficient for correct MMD simulation. For example, if the assembly is comprised by 10^8 initiator molecules, which corresponds to the assembly of 10^{12} monomer molecules, then a 1-hour simulation of MMA polymerization totalled 25 minutes, which is significantly faster than in [4], in which the above-mentioned process took 2 hours run time (on a much more powerful IntelCore i5 (2 cores, 3.46 GHz, 16 GB) computer) while the assembly was characterized as containing 10^{11} monomer molecules. Thus, the calculating program, being the result of the study, is believed to be over 50 times as efficient.

The Hui-Hamielec model parameter determination

The values of the coefficients A_1, A_2, A_3 for the mass radical polymerization of styrene can be found in [8]. An indispensable condition for this process is thought to be the monotonic decrease in the chain termination rate as the conversion increases. The values of the Hui-Hamielec model parameters for MMA radical polymerization were determined in [32] by solving the inverse problem, along with varying the Hui-Hamielec coefficients and chain growth reaction rate. The task was to achieve matching of experimental and calculated dependences of the MMA conversions in the presence of AIBN initiator within a temperature range of 50–80°C at different initial concentrations of the initiator. It was found that the inverse problem has several solutions (sets) that describe the experimental conversions being characterized by virtually the same correlation coefficient. Firstly, some sets belonging to high conversions area lead to the increase in k_t. These sets were ruled out from the solution as having no physical meaning. Secondly, it was found that the $k_t(x)$ dependence has an intersection point at different temperatures (Pic. 3b). Therefore, the sets, their intersection point being found in the conversion domain x<1, were also excluded. As a result, the following solution was determined:



Pic. 3. Chain termination rate dependence on conversion at different temperatures of MMA polymerization

The Hui-Hamielec model coefficients (8) were applied to take the gel effects into account while simulating the MMA mass radical polymerization by the MC method.

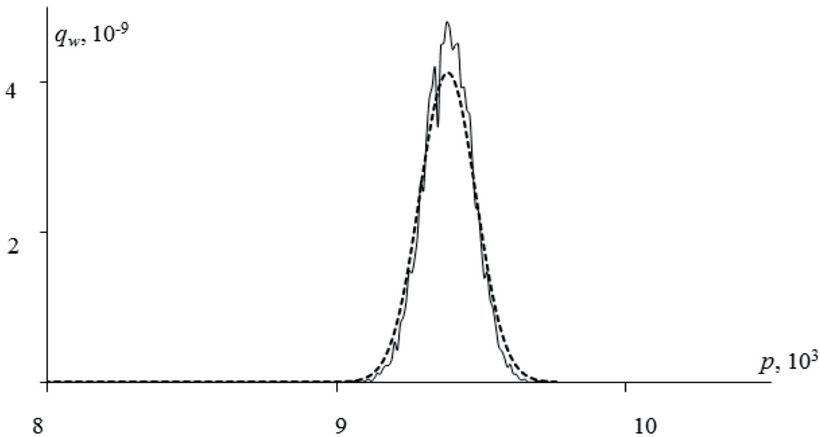
Program testing

In order to test the simulation program for the MMA mass radical polymerization by the MC method computational experiments were carried out for certain extreme cases.

Having performed the intact macromolecules growth simulation with no transfer or chain termination reactions, the expected MMD was obtained that can be described by the Poisson distribution function (Pic. 4):

$$q_w(p) = \frac{p}{\overline{P}_n} \frac{(\overline{P}_n)^p}{p!} \exp(-\overline{P}_n), \qquad (9)$$

where p is polymerization degree, $\overline{P}_n$ is number-average polymerization degree.

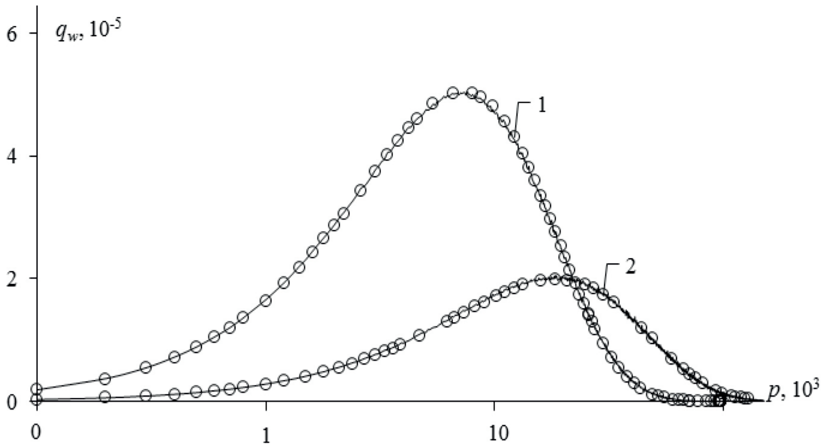


Pic. 4. MMP, obtained as a result of the chain growth reaction rate simulation: dashed line is used to denote the Poisson distribution (9), while solid line denote what was obtained by the MC simulation at t=10 c, k_p=100 L/(mol·sec), the assembly size being 100 mln., T=70°C, $[AIBN]_0$=1 mmol/L

It is known, that the chain growth, growing chain transfer and/or radical disproportioning reaction should result in MMD formation being correspondent to the Flory distribution function:

$$q_w(p) = \frac{p}{\overline{P}_n^2} \exp(-\frac{p}{\overline{P}_n}) \qquad (10)$$

It is but true, that the type of MMD obtained as a result of chain growth reaction rate and chain transfer to monomer simulation is the Flory distribution (Pic. 5, curve 1), whereas the chain growth reaction rate, chain transfer to monomer and radical disproportioning simulation leads to the same result (Pic. 5, curve 2).

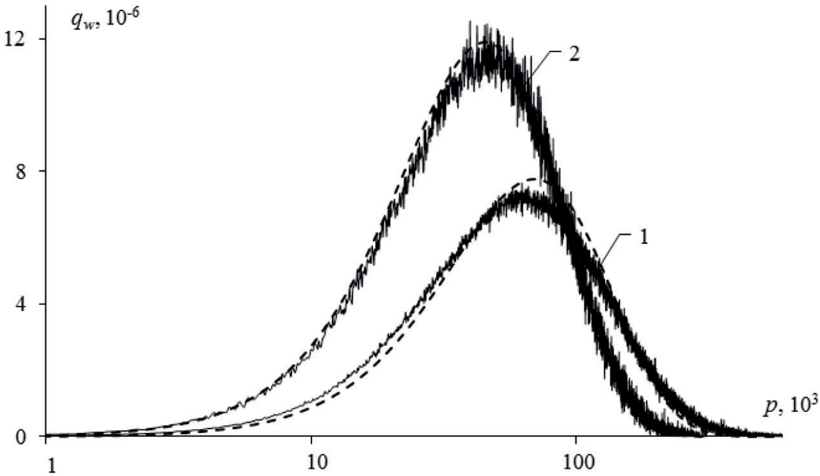


Pic. 5. PMMA MMD: ○ – the Flory distribution (10), solid lines – MC (the assembly size – 50 mln., T=70°C, $[PBO]_0$=1 mmol/L, k_p=670 L/(mol·sec), k_m =0.035 L/(mol·sec)), 1 – chain growth reaction rate and chain transfer to monomer simulation (t=190 c); 2 – chain growth reaction rate, chain transfer to monomer and radical disproportioning simulation (t=6600 c, k_{disp} (Table 2))

In case only chain growth and radical recombination reactions are observed or radical recombination prevails over chain transfer to monomer, then, as a result, the type of MMD should be formed, the one described by the Schulz distribution:

$$q_w(p) = \left(\frac{2}{\overline{P}_n}\right)^2 \frac{p^2}{\overline{P}_n} \exp(-\frac{2p}{\overline{P}_n}) \tag{11}$$

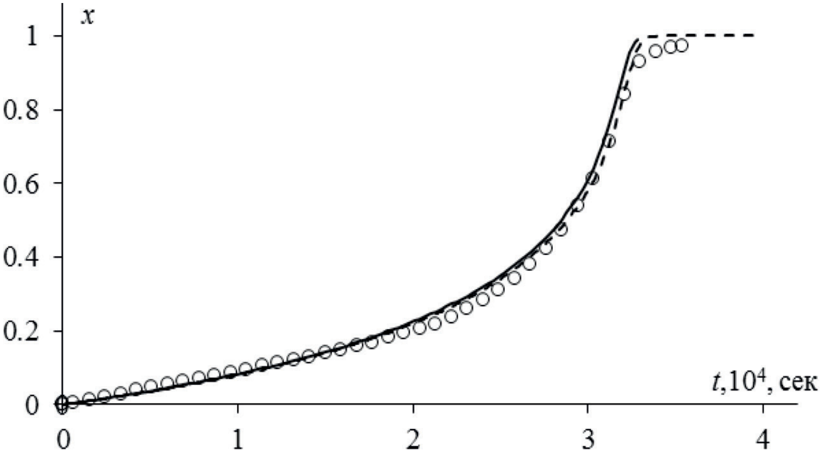
In this asymptotic case, the program testing was also proved successful (Pic. 6).



Pic. 6. PMMA MMD, dashed lines – the Schulz distribution (11), solid lines – MC (the assembly size – 50 mln., T=70°C, $[PBO]_0$=1 mmol/L, k_p=670 L/(mol·sec), t=1 ч, k_{com} (Table 2)): 1 – chain growth reaction rate and radical recombination; 2 – chain growth reaction rate and chain transfer to monomer simulation (k_m=10^{-4} л/(mol·sec)) and radical recombination

To test the MC results, the system of differential equations (1–3) was solved using the RK4 method for the case of MMA polymerization along with the presence of PBO having initial concentration of 1 mmol/L at T=60°C. The results of the system solution, that was carried out using both the methods, correlated to a full extent (Pic. 7).

Thus, the test results show that the program that was developed to simulate substance initiated radical polymerization by the MC method taking the gel effect into account according to the Hui-Hamielec model is capable of correct reproduction of both monomer conversion variation and MMD while polymerization is in progress.

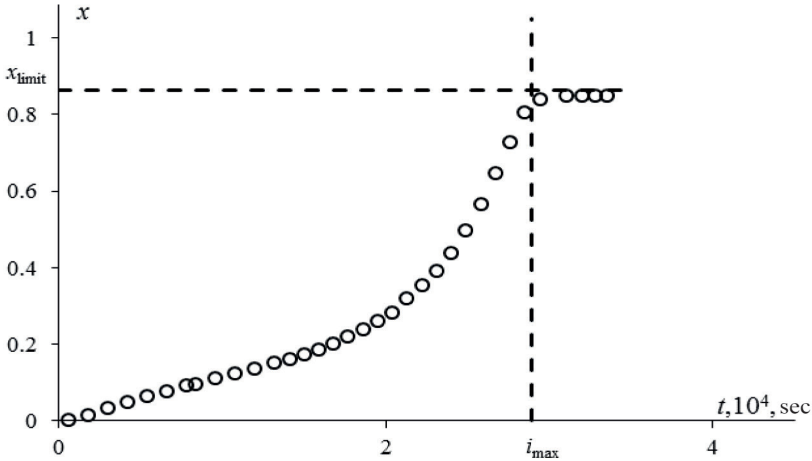


Pic. 7. MMA conversion dependency: solid line – MC method, dashed line – RK4, ○ – experimental data ($[PBO]_0$=1 mmol/L, 60°C)

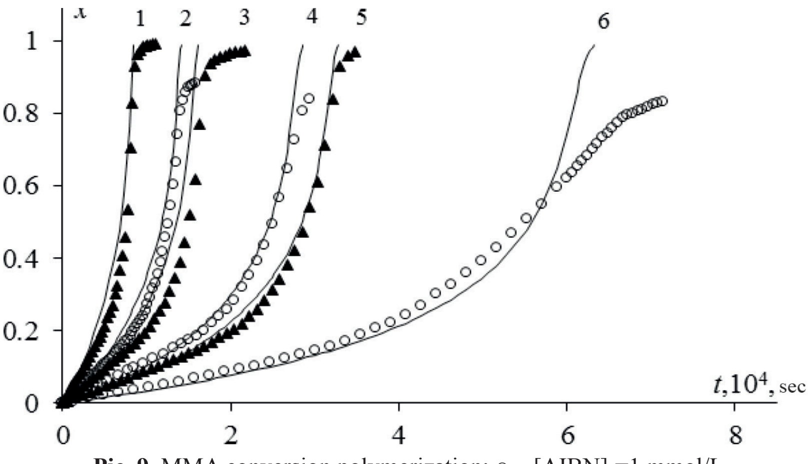
Conversion dependencies

The strategy of determining the chain growth reaction rate was to solve the inverse problem by approximating the MMA experimental conversion dependencies in the presence of AIBN initiator at its different initial concentrations. That is, one needs to minimize the functional:

$F(k_p) = \sum_{i=1}^{i_{\max}} (x_i^{\exp er} - x_i^{calc})^2$, where i is the number of the actual data point being relative to the $i_{\max}$ value selection. The MMA experimental conversion dependencies never achieve theoretically maximum possible value of x=1, but only tend to reach a certain limit value of x_{limit}<1 (Pic. 8). This is explained by PMMA glass transition in the high conversions area [11, 33–34], in which all of the reactions change to a diffusion mode (I). The theoretical description of the glass transition within the MMA polymerization process is thought to be possible provided the additional kinetic parameters are introduced into the model [34–35], which complicates the model. Therefore, we have limited the $i_{\max}$ to exclude the glass transition area.



Pic. 8. MMA experimental conversion dependency on polymerization time ($[AIBN]_0$=1 mmol/L, T=60°C)

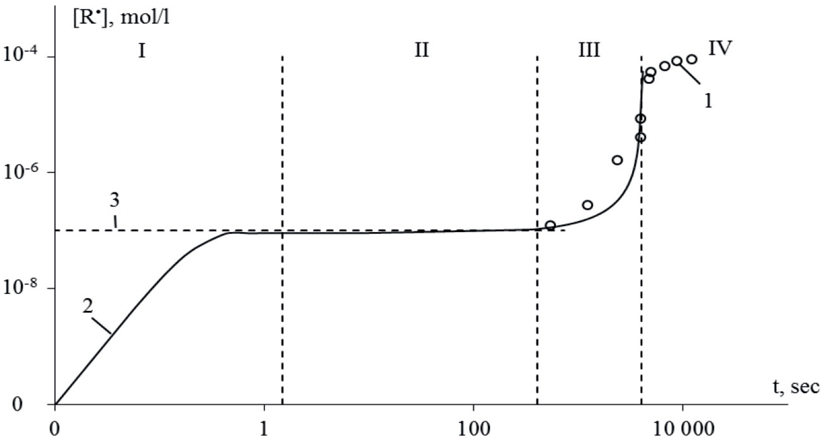


Pic. 9. MMA conversion polymerization: ○ – $[AIBN]_0$=1 mmol/L, ▲ – $[PBO]_0$=1 mmol/L; 1 – 80°C; 2,3 – 70°C; 5,4 – 60°C; 6 – 50°C; symbols – experimental data, lines – obtained by the MC simulation

The chain growth reaction rate was determined using the experimental data corpus on MMA radical polymerization in the presence of AIBN initiator, then it was tested using the PBO initiator. The convincing correlation of estimated and experimentally observed conversion curves (Pic. 9). The parameter k_p=2.5·10^6·exp(–2823/T), L/(mol·sec) (Pic. 2) corresponds to the k_p value range [12] (Table 1).

Macroradicals concentration

Only one [29] work contains data on experimentally measured macroradicals concentration within the MMA polymerization process carried out at 60°C in the presence of AIBN with the initial concentration of 100 mmol/L. The work also contains the dependence $y(t)$=[$R^•$]/M, which in the coordinates [$R^•$](t) is almost identical to the radicals concentration within the MC simulation (Pic. 10, 1–2), which again confirms adequacy of the Hui-Hamielec model in case of the MMA polymerization.

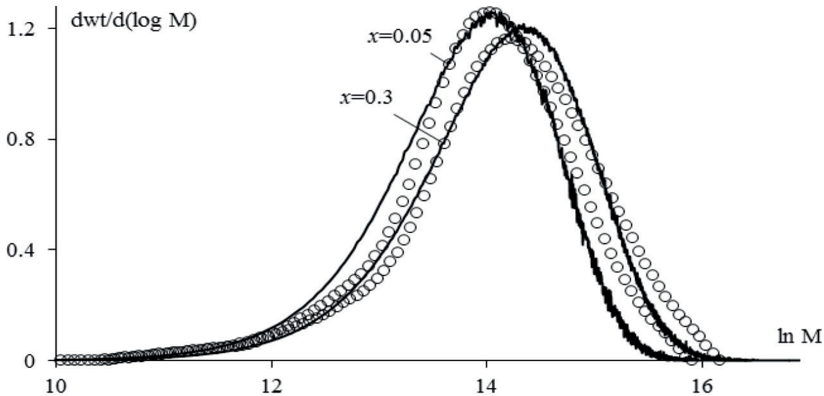


Pic. 10. Macroradicals concentration dependency on the MMA polymerization: 1 – experiment [2], 2 – the MC simulation (60°C, [AIBN]$_0$ = 100 mmol/L, k_p = 520 L/(mol·sec) likewise), 3 – quasi-steady approximation (k_p = 660 L/(mol·sec))

There are four main sections in the kinetic curve: I – the initial section of the concentration increase up to the steady-state value, II – the section with a constant concentration of macroradicals, III – the section on which there is a sharp increase in the macroradicals concentration, IV – the glass transition section. Note that the length of the first two sections is quite small compared to the polymerization time section. Almost all of the monomer gets polymerized within sector III, whereas on section IV all polymer reactions slow down because of all the glass transition.

PMMA MMD

Thus, the chain growth reaction rate was determined on the first stage of the inverse problem solution On the second stage the transfer to monomer reaction rate was determined using the correlation of estimated and experimentally observed values (at 50–70°C) of average molecular masses and MMD (Pic. 11). Having approximated the k_m value, k_m=2.79·10^5·exp(-5450/T), L/(mol·sec) was determined.



Pic. 11. Typical PMMA MMD: symbols – experimental values (T=70°C, $[PBO]_0$=1 mmol/L), solid line – what was obtained by the MC simulation at k_p =670 L/(mol·sec), k_m=0.035 L/(mol·sec)

Thus, it is the algorithm of the substance initiated MMA mass radical polymerization taking the gel effect into account according to the Hui-Hamielec model that was developed [8] as well as the model parameters were determined.

Conclusion

The chain growth reaction rate in quasi-steady approximation as well as by the MC method was determined for the purposes of MMA mass radical polymerization in the presence of both AIBN and PBO within the temperature range of 50–90°C. The use of quasi-steady approximation results in significant increase of the rate. Due to this, the gel effect should be taken into account, that was performed while simulating the MC. The chain growth reaction rate value, obtained as a result of the simulation process, is thought to be more correct.

The pertinent theoretical model of the substance initiated MMA mass radical polymerization taking the gel effect into account according to the Hui-Hamielec model was developed.

The original algorithm was created to simulate radical polymerization using the MC method as well as the software was developed that enables to spend adequate run time to calculate reagent concentration at various polymerization periods, speed of the simulated reactions, polymer MMD and average MM values. One of the most significant advantages of the developed algorithm of radical polymerization simulation is thought to be the fact that it can be easily modified by adding new block to the program thus making it possible to simulate other reactions.

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