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RESEARCH ARTICLE

Computer modeling of the synthesis of styrene–butadiene rubber: Influence of the feed of a chain transfer agent on the characteristics of the product

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Abstract

Objectives. To develop mathematical approaches and algorithms for analyzing the influence of various methods for feeding a chain transfer agent to a cascade of reactors, taking into account the choice of feed points on the characteristics of the final product of copolymerization using computer modeling.

Methods. The processes of synthesis of copolymers were mathematically modeled using a statistical approach (Monte Carlo method). The developed algorithm is based on calculating the probabilities of elementary reactions in the process under study. In the case of continuous production of the copolymer in a cascade of reactors, it must be taken into account that the residence time of each particle of the reaction mixture in the reactor is subject to a probability distribution. The algorithm models the formation of copolymer macromolecules at the particle level, permitting the average molecular characteristics of the copolymer to be calculated and its microstructure to be studied based on modeling results.

Results. The dependencies of the intrinsic viscosity on the reactor number and conversion were constructed by means of mathematical modeling. The calculation results showed satisfactory agreement with the experimental data obtained in production. The dependencies of the molecular weight distribution of the copolymer, the weight-average molecular weight, and the microheterogeneity index on the reactor number were constructed for various methods of feed of the chain transfer agent, i.e., to two and/or three points of the reactor cascade. The modeling and calculation results confirmed the influence of the method of adding the chain transfer agent to the cascade reactors on the molecular characteristics of the copolymer.

Conclusions. The analysis of the structure of the molecular units of the styrene–butadiene copolymer showed a decrease in the weight-average molecular weight of the final product and an increase in its stiffness in the case of the three-point feed of the chain transfer agent.

Keywords

copolymerization, reactor cascade, butadiene, styrene, tertiary dodecyl mercaptan, statistical modeling, Monte Carlo method, molecular weight distribution, polydispersity, microheterogeneity

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НАУЧНАЯ СТАТЬЯ

Компьютерное моделирование процесса синтеза бутадиен-стирольного каучука: влияние подачи регулятора на характеристики продукта

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Аннотация

Цели. Развитие математических подходов и алгоритмов анализа влияния различных способов подачи регулятора в каскад реакторов с учетом выбора точек подачи на характеристики конечного продукта процесса сополимеризации с применением компьютерного моделирования.

Методы. При математическом моделировании процессов синтеза сополимеров применялся статистический подход (метод Монте-Карло). Разработанный авторами алгоритм основан на вычислении вероятностей осуществления элементарных реакций исследуемого процесса. В случае непрерывного производства сополимера в каскаде реакторов необходимо учитывать, что время пребывания каждой частицы реакционной смеси в реакторе подчиняется вероятностному распределению. Реализация алгоритма позволяет имитировать образование макромолекул сополимера на уровне частиц, что дает возможность вычислять его усредненные молекулярные характеристики и исследовать микроструктуру на основе данных, полученных в результате моделирования.

Результаты. Методами математического моделирования построены зависимости характеристической вязкости от номера реактора и конверсии. Результаты расчетов показали удовлетворительное согласование с экспериментальными данными, полученными на производстве. Построены зависимости молекулярно-массового распределения сополимера, среднемассовой молекулярной массы и коэффициента микрогетерогенности от номера реактора для различных режимов подачи регулятора — в две и/или три точки каскада реакторов. Анализ результатов моделирования и расчетов подтвердил влияние способа добавления регулятора в реакторы каскада на молекулярные характеристики сополимера.

Выводы. Анализ структуры молекулярных звеньев бутадиен-стирольного сополимера показал снижение среднемассовой молекулярной массы конечного продукта и увеличение его жесткости при трехточечном режиме регулирования процесса.

Ключевые слова

сополимеризация, каскад реакторов, бутадиен, стирол, третичный додецилмеркаптан, статистическое моделирование, метод Монте-Карло, молекулярно-массовое распределение, полидисперсность, микрогетерогенность

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INTRODUCTION

In modern industry, the production of synthetic materials, in particular, rubber is one of the key industries which contribute to progress in various fields, such as the automotive industry, chemical industry, medicine, among others. However, there is an urgent need for the development, modification, and optimization of technological processes requiring many factors and parameters to be considered in their production.

Natural rubber does not have the qualities necessary for the creation of high-quality rubber products. Therefore, a wide variety of types of synthetic rubber are produced. It is synthesized under industrial conditions by polymerization/copolymerization processes [1]. The resulting product, unlike natural rubber, is resistant to environmental damage, highly elastic, and can withstand low temperatures. The material formed in the process is subsequently processed into rubber by vulcanization.

Styrene–butadiene synthetic rubber from the group of general-purpose rubbers is the most widely used in comparison with other large-tonnage rubbers. In world production, its fraction is slightly more than 30%. It is used in the production of various rubber products (car mats, hoses, shoe soles, cable insulation, etc.), with the main area of application being the production of tires, mainly for passenger cars [2].

Synthetic rubbers based on butadiene and styrene are synthesized by free-radical styrene-butadiene copolymerization in an aqueous emulsion. This process is carried out at low temperatures (5–6°C) in a continuous mode in several reactors simultaneously combined into a cascade of 9–12 stirred-tank reactors, shown in Fig. 1, as a component of the production scheme. In this case, the flow of the reaction mixture is continuously fed into the first reactor of the cascade, and the reaction products are removed from the last reactor [3]. The described approach to carrying out the process significantly reduces the operating costs of the reactors, extends the overall service life, and ensures the stability of the technological process and, consequently, the stability of the manufactured product [4].

One of the important process parameters affecting the properties of the polymer product is the feed mode of the chain transfer agent (CTA), i.e., its quantity, feed rate, feed points, and feed time. Changing the CTA feed mode can significantly affect the molecular weight, structure, and properties of the formed product, which are directly related to its performance [5].

Mathematical modeling of polymerization and copolymerization processes plays an important role in studying their various aspects and, accordingly, their optimization [6]. Research based on constructing a mathematical model is focused on calculating the characteristics of the formed copolymer and the product obtained, as well as finding optimization modes for controlling the process parameters, and analyzing their mutual influence under industrial production conditions [7].

This work aims to study the effect of various CTA feed modes in a cascade of reactors on the characteristics of the copolymer product by computer modeling of the process. Computational experiments based on a computer model may significantly reduce the costs of conducting experiments under laboratory and, particularly, industrial conditions in real time.

EXPERIMENTAL

Previously [8, 9], we proposed an algorithm for modeling the copolymerization process performed in a continuous mode in a cascade of reactors. This algorithm is based on the Monte Carlo method according to the approach proposed by Gillespie [10, 11]. The basis of the algorithm is a cycle of the following stages implemented at certain points in times:

- calculation of reaction rates at a current ratio of particles in the reactor;
- calculation of the probabilities of their implementation based on the values of the rates and their sequential arrangement on the interval [0, 1];
- generation of a random number on the same interval, determination of the part of the interval that contains the random number, and selection of the corresponding part of the reaction interval;
- modeling the selected reaction at the level of change in the number of types of particles of the reaction

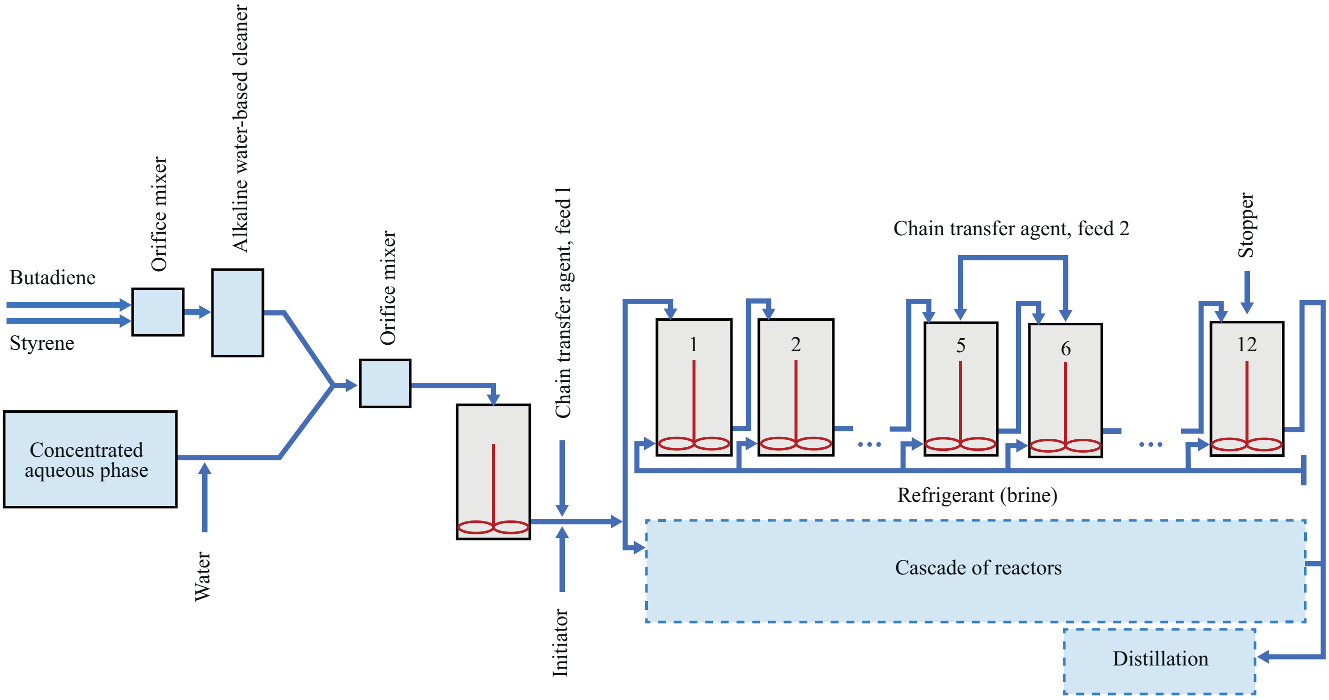

Fig. 1. Scheme of continuous production of synthetic rubber by emulsion copolymerization of butadiene with styrene

mixture (e.g., an increase in the length of growing macromolecules and a decrease in the number of monomers when modeling the growth reaction, etc.).

The condition for stopping the cycle is reaching a certain condition, e.g., achieving a predetermined value of monomer conversion.

Since the synthesis of styrene–butadiene rubber under industrial conditions is performed continuously in parallel in several cascade reactors, it should be noted that each component of the reaction mixture has its own residence time in the reactor. Within the framework of the proposed model, the residence time is a random variable characterized by the probability distribution function $p(t)$ [12].

The probability of which reactions can occur in each of the cascade reactors at a specific point in time depends directly on the types of particles of the reaction mixture (monomer, initiator, CTA, copolymer macromolecules) and the quantities in these reactors.

With the reaction selected for modeling, the time of its implementation is put in correspondence:

$$\Delta t = \frac{1}{R_{\text{sum}}} \ln\left(\frac{1}{r_p}\right),$$

wherein R_{sum} accumulates the rates of all elementary reactions that can occur and the probability of which is not zero, and r_p is a random number generated on the interval [0, 1].

The probability of an event, i.e., the presence of the particle under study in the cascade reactor under consideration during the time from t to $t + dt$, is given by the value $p(t)dt$. The function $p(t)$ depends on the type of reactor used in the process technology. In our case, the reactors in the cascade are continuous stirred-tank reactors, and $p(t)$ is represented as

$$p(t) = \left(\frac{n}{\tau}\right)^n \frac{t^{n-1}}{(n-1)!} e^{-\frac{nt}{\tau}}, \tag{1}$$

wherein τ is the average residence time of particles of the reaction mixture in one reactor, h; and n is the number of devices in the reactor cascade [13].

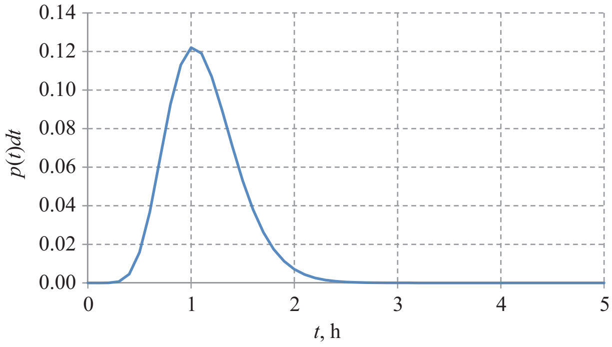

Fig. 2. Residence time distribution in a cascade of 11 reactors

Figure 2 shows the residence time distribution of the components of the reaction mixture in a cascade of 11 reactors 10.8 m^3 in volume each at a volume flow rate of C_f = 9.5982 m^3/h. At these parameters, the average residence time of particles of the reaction mixture in one reactor is 1.125 h, which corresponds to the peak of the curve in Fig. 2.

In order to model the copolymerization process in a cascade of continuous stirred-tank reactors, the residence time in the current reactor needs to be defined for each component of the mixture (molecule and macromolecule) using distribution (1). For the time interval from 0 to $t_{\max}$, a partitioning step dt is selected in such a way that the events corresponding to all residence time variants form a complete group of events. In the case considered in Fig. 2, such a time interval is the interval from 0 to 5 h with a step of 0.1 h.

In order to determine the residence time of each individual particle of the reaction mixture in the reactor under consideration, a new random value is generated from the interval [0, 1], and the value of f is selected in such a way that the following inequality is satisfied:

$$\sum_{i=1}^{f-1} p((f-1)\cdot dt) < r_p < \sum_{i=1}^{f} p(f \cdot dt).$$

This inequality characterizes the part of the interval in which the generated value is located. Accordingly, for the particle in question, the residence time in the current reactor is defined as $f \cdot dt$. Therefore, the time of transfer of particles of the reaction mixture to the next reactor after their residence time in the current reactor has expired needs additionally to be monitored.

As a result, the formation of the copolymer in the cascade of series-connected reactors is modeled. The model considers the constant flow of the initial mixture of particles of various types into the first reactor and the removal of the formed copolymer. This approach to considering molecules of the mixture and macromolecules of the product at the particle level allows us to proceed to calculate the molecular-weight and viscosity characteristics of the product.

Data on all particles involved in the process, including those formed in it, can be obtained at any time, upon reaching specific values of monomer conversion, as well as at the outlet of each reactor. Such an approach allows us to obtain the following information for each reactor:

- the number of particles of each monomer, initiator, and CTA;
- the numbers of active and inactive macromolecules of each type, the chain length, and the structure of the composition of each of them. If we additionally save data on which two or three chain links are at the end,

we can describe which types of dyads and triads of links make up the structure of macromolecules of the compound through their fractions;
- molecular-weight characteristics (number-average molecular weight M_n, weight-average molecular weight M_w, and molecular weight distribution) and viscosity characteristics (intrinsic viscosity and Mooney viscosity) of the copolymer product [14, 15].

RESULTS AND DISCUSSION

We created a program for conducting computational experiments. The approach presented was used to calculate the process of copolymerization of butadiene with styrene in several continuous stirred-tank reactors, sequentially forming a cascade (in the C# and Visual C++ environment).

By means of computational experiments, we evaluated the influence of the composition of the reaction mixture or the feed modes of various reagents on the properties of the resulting copolymer or the product produced from it. In particular, we considered the effect of the CTA feed mode on these properties by the example of conducting the process in a cascade of 11 continuous stirred-tank reactors at the following characteristics of the loaded mixture:

- mass flow rate of monomers—3.5 t/h (100 parts by weight per hour (pts. wt/h); 70 and 30 pts. wt/h for butadiene and styrene, respectively);
- initiator (pinane hydroperoxide)—0.054 pts. wt/h;
- water : monomer ratio = 220 : 100;
- working volume of reactor—10.8 m^3;
- volume flow rate—9.5982 m^3/h.

The experimental data at the given process characteristics (Table) were obtained at the Central Laboratory of *Sterlitamak Petrochemical Plant* (Sterlitamak, Bashkortostan, Russia) [8]. The molecular weight of the copolymer was controlled by an CTA as *tert*-dodecyl mercaptan, fed at several points of the reactor cascade. The CTA was continuously fed to the first reactor at a mass flow rate of 0.125 pts. wt/h and to the third and sixth reactors at a mass flow rate of 0.027 pts. wt/h.

Computational experiment 1 was carried out according to the approach we proposed, modeling 30 h of the process with the above characteristics. The results obtained were compared with the results of the production experiment (Table).

Figure 3 presents the profiles of the intrinsic viscosity of the copolymer along the reactor cascade. Figure 4 shows the dependence of the intrinsic viscosity of the copolymer on the total conversion of monomers. At the outlet of the first reactor of the cascade, the discrepancy between the result of the computational experiment and the production data was maximum (30%) At the outlet of the last reactor of the cascade, the discrepancy was 3.6%, which demonstrated the agreement between the computational and production data.

Table. Results of production experiment

Reactor number	Mooney viscosity	Intrinsic viscosity, dL/g	Monomer conversion, %
1	–	0.73	5.5
2	–	–	14.1
3	–	0.86	23.7
4	–	1.28	29.6
5	–	1.28	32.0
6	–	–	41.8
7	38	1.66	51.3
8	–	1.70	55.8
9	79	2.24	64.0
10	–	2.31	69.0
11	87	2.42	70.4

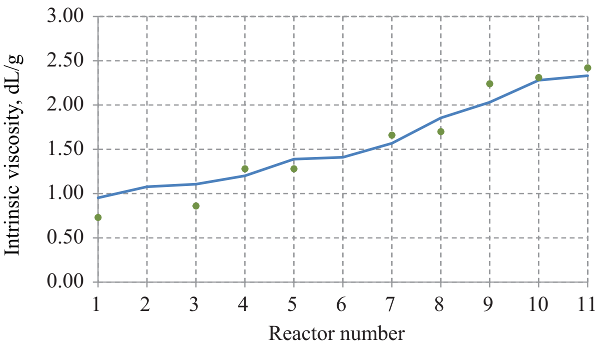

Fig. 3. Dependencies of the calculated (line) and experimental (points) values of intrinsic viscosity along the reactor cascade

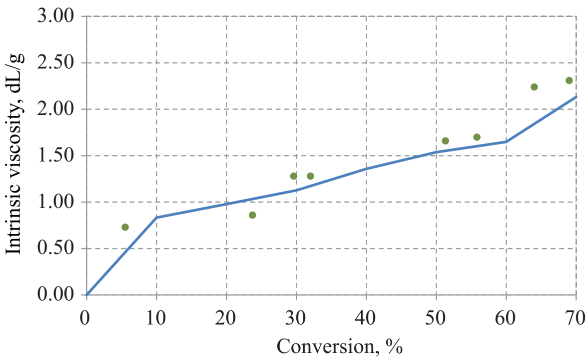

Fig. 4. Dependencies of the calculated (line) and experimental (points) values of intrinsic viscosity on conversion of monomers

The behavior of the intrinsic viscosity curve of the resulting copolymer is controlled by the change in the amount of the CTA in the cascade reactors (Fig. 5). More than half of the loaded portion of the CTA is consumed in the first and second reactors. This significantly slows down the increase in the intrinsic viscosity therein when compared with the reactors of the second half of the cascade.

The CTA is additionally fed for the second time to the third reactor, and for the third time to the sixth reactor of the cascade. As a result, it can be observed that the intrinsic viscosity of the product changes slowly: from 1.10 dL/g in the third reactor to 1.41 dL/g in the sixth reactor. However, due to the active consumption of CTA particles and, accordingly, the smaller amount in the last reactors of the cascade, an active increase in the molecular weight and intrinsic viscosity of the copolymer can be observed.

A similar change can also be observed in the curve demonstrating an increase in the copolymer polydispersity (the ratio of the weight-average molecular weight to the number-average molecular weight) with an increase in the reactor number (Fig. 6). The polydispersity in the cascade reactors changes in the range from 2 to 4.3, which complies with standards for styrene–butadiene rubber synthesized by low-temperature free-radical copolymerization [3].

The molecular weight distribution describes the proportions of macromolecules with different molecular weights in the copolymer. To construct this distribution using data on all chains of the formed copolymer obtained in the computational experiment, by analogy with gel chromatography, the “dead” macromolecules of the copolymer that have left the last reactor of the cascade need to be fractionated. For this purpose, we form groups (fractions) in which the molecular weights of macromolecules differ by ΔM. Then, for each group formed, we calculated the ratio of the sum of the molecular weights of macromolecules in the group to the sum of the molecular weights of macromolecules in all groups is, i.e., the weight fraction of the group, which must be normalized by dividing the obtained value by ΔM [8]. In the case under consideration, the curve presenting the change in the normalized weight fraction with an increase in the group weight is shown in Fig. 7 at two time points: after 15 and 30 h of process modeling.

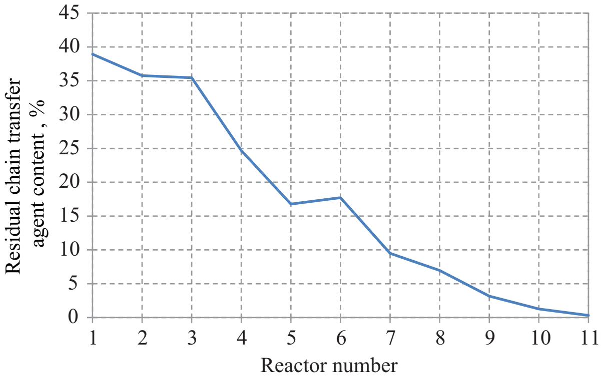

Fig. 5. Dependence of the calculated residual CTA content along the reactor cascade

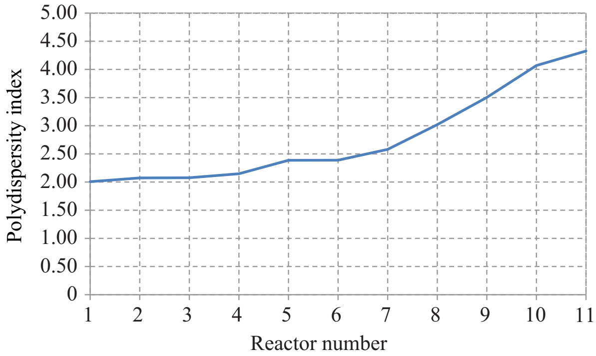

Fig. 6. Calculated polydispersity dependence along the reactor cascade

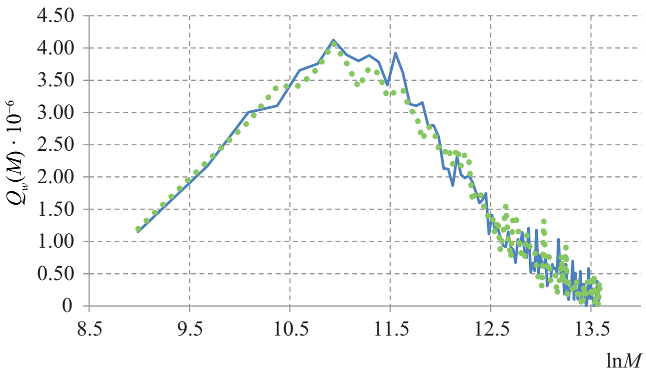

Fig. 7. Differential molecular weight distribution curve of the copolymer after 15 h (dotted line) and 30 h (solid line) of process modeling

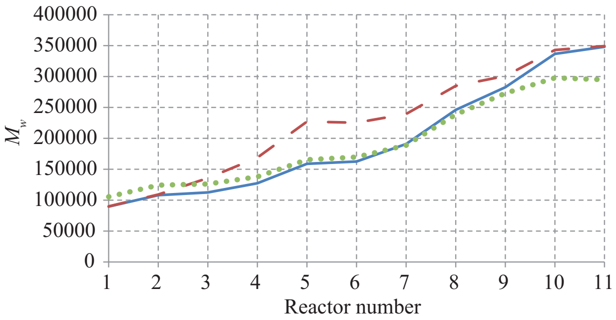

Fig. 8. Dependencies of the weight-average molecular weight along the reactor cascade

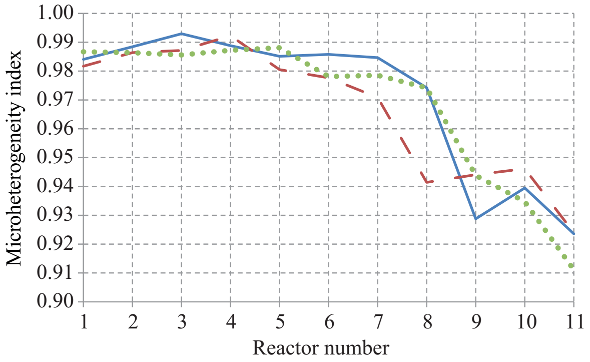

Fig. 9. Dependencies of the microheterogeneity index of the copolymer along the reactor cascade

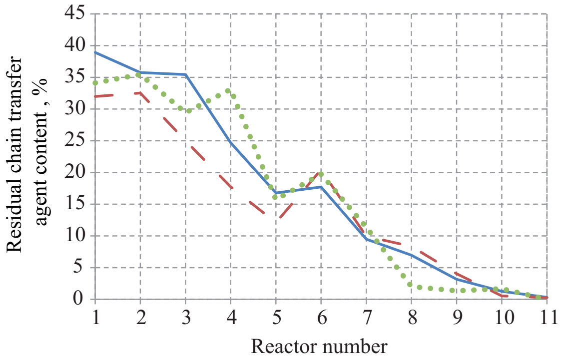

Fig. 10. Calculated residual CTA content dependencies along the reactor cascade

The proposed approach to modeling and the program developed on its basis permits the microstructure of the copolymer changes to be studied when changing the technological scheme of the copolymerization process under industrial conditions or when varying the process characteristics. Thus, the sequences in which butadiene and styrene units are linking together in macromolecules can be studied. Further in the work, we considered additional modes of continuous feed of the CTA and their effect on the product properties, while maintaining its total amount at the same level:

- to two points with a larger amount of the CTA in the second half of the reactor cascade: the first point (reactor 1), 0.125 pts. wt/h; and the second point (reactor 6), 0.054 pts. wt/h (computational experiment 2);
- at three points with a different CTA distribution: the first point (reactor 1), 0.109 pts. wt/h; the second point (reactor 3), 0.035 pts. wt/h; and the third point (reactor 6), 0.035 pts. wt/h (computational experiment 3).

In the figures below, the solid lines show the dependencies for the three-point mode of feeding the CTA in the production experiment (computational experiment 1); the dashed lines, the two-point mode of feeding the CTA (computational experiment 2); and the dotted lines, the three-point mode of feeding the CTA with a different distribution of the CTA (computational experiment 3).

Figures 8 and 9 demonstrate the profiles of the weight-average molecular weight of the copolymer and the microheterogeneity index along the reactor cascade in the above modes of feeding the CTA. Figure 10 presents the dependence of the residual CTA content along the reactor cascade for each of the modes.

Figures 11–13 show the dependencies of the fractions of various types of dyads in copolymer macromolecules along the reactor cascade in the modes of feeding the CTA to the first, third, and sixth reactors of the cascade in accordance with the experimental design at the production facility.

Thus, changing the mode of feeding the CTA to the reactor cascade (choosing the feed points) affects the characteristics of the formed copolymer. The three-point feed of the CTA helps to reduce the weight-average molecular weight of the formed product, narrow the spread of microheterogeneity index, and a corresponding decrease in the tendency to form long blocks in the copolymer.

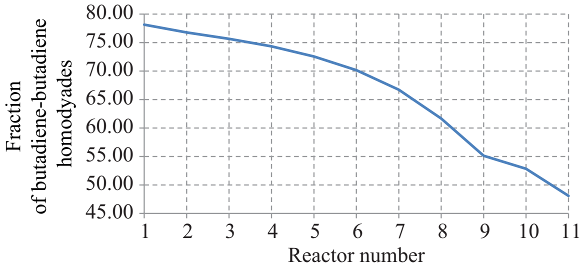

Fig. 11. Dependence of the fraction of butadiene–butadiene homodyads in copolymer chains along the reactor cascade

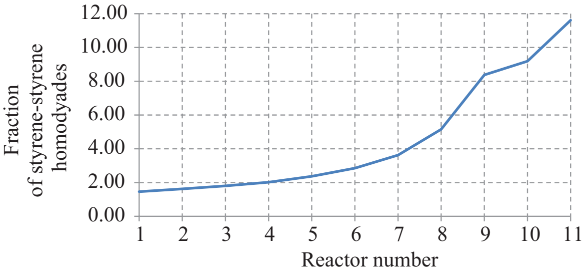

Fig. 12. Dependence of the fraction of styrene–styrene homodyads in copolymer chains along the reactor cascade

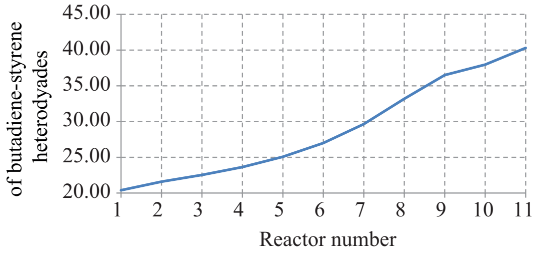

Fig. 13. Dependence of the fraction of butadiene–styrene heterodyads in copolymer chains along the reactor cascade

CONCLUSIONS

Thus, the proposed approach based on modeling the formation of butadiene–styrene copolymer macromolecules using the Monte Carlo method adequately describes its production in a cascade of continuous stirred-tank reactors. Thanks to the information obtained by the modeling, the molecular-weight and viscosity properties of the formed copolymer in dynamics at a constant feed flow rate under various production conditions can be studied. This allows the influence of the production mode to be assessed. Based on the results of the computational experiments, it was noted that, with an increase in the process time, the fraction of high-molecular-weight fractions of the copolymer increases. This occurs due to an increase in the content of styrene homodyads in the forming copolymer chains. This, in turn, renders the product produced from it less elastic. Fractional feeding of the CTA to three reactors helps to reduce the molecular weight of the final product, narrow the spread of microheterogeneity index, and, as a result, decreases the probability of the formation of long blocks in the copolymer.

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Authors' contribution

All authors equally contributed to the research work.

The authors declare no conflict of interest.

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