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Development of a Cloud Service for Comprehensive Research of Polymer Synthesis Processes

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Abstract

The issue of digitalization in chemical technology production is currently quite pressing, and the available computational infrastructure is insufficient for assessing the technological properties of the products obtained through mathematical modeling tools. This problem is particularly relevant for polymer synthesis processes, where standard empirical evaluations require enormous computational resources, and existing methods and algorithms prove ineffective when organizing multiple computational trials to select optimal production scenarios. The aim of this study is to develop a cloud-based digital service that enables comprehensive research into complex physicochemical processes occurring via polymerization mechanisms. The implementation of all algorithms is based on the use of kinetic and statistical approaches to modeling, and the embedded calculation methods are adapted to the specifics of polymerization processes. The conceptual framework of the developed cloud service is represented by a three-tier network architecture, and the established mechanism of network interaction allows the service to operate in a 24-hour multi-user mode. Task execution in the remote environment and the distribution of computational resources are handled using Docker containerization technology, which provides software-level virtualization within the operating system. The storage subsystem is managed by the MongoDB database management system, which supports distributed information storage functions. The organization of test computational experiments in evaluating the detailed properties of polymer products allowed for the assessment of the system's core logic in web interface mode and the adequacy of the obtained calculation results.

Keywords:

Cloud Computing; Polymer; Algorithm; Network; Modelling; Management Systems.

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1- Introduction

In the chemical engineering sector, tasks related to improving product quality technology and increasing production profitability, which can be characterized as a complex physicochemical system operating under the influence of various chemical, physicochemical, and hydrodynamic phenomena and effects, are increasingly being set. The application of mathematical models and methods to describe these effects allows for comprehensive research of complex processes and determines the quantitative relationship between the composition of the reaction mixture, production conditions, and the properties of the resulting product.

A classic example of complex systems characterized by significant non-stationarity and challenging analysis is polymer synthesis processes. The intricate structure of the resulting high-molecular-weight compounds and the non-trivial nature of the elementary reactions necessitate the use of efficient modeling methods. The mathematical description for the known reaction mechanism is based on kinetic [1-3] and statistical [4-6] modeling approaches. The kinetic

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approach involves the development of mathematical models that describe the changes in the concentration of various system components over time, represented as a system of ordinary differential equations, followed by their numerical solution. Unfortunately, the range of predicted properties is limited to average molecular characteristics [7], and detailed product properties at the macromolecular level cannot be achieved within the framework of the kinetic approach. The statistical approach is based on the use of probabilistic laws to describe and analyze various aspects of polymerization processes. The data obtained through the statistical approach are highly detailed but are only valid when a sufficiently large number of computational trials are conducted [8].

The description of processes at the scale of large-scale industrial production further complicates the modeling and necessitates consideration of the continuous flow of reactants and products through the reactor, including the dynamics of parameter changes over time and space [9]. In the framework of the kinetic approach, this requires the inclusion of appropriate recurrent relationships in the mathematical description, which define the mass transfer during the reaction process [10]. When modifying the statistical approach, it becomes necessary to constantly account for the parameters characterizing the position of the modeled macromolecules in each reactor within the cascade [11], leading to a significant increase in the volume under consideration. Consequently, the organization of computational trials for the empirical evaluation of the product demands enormous computational resources and is virtually impossible when setting and solving optimization tasks using the statistical approach.

Similar challenges arise when addressing the task of finding optimal production modes. Most scientific research in this area focuses on using analytical representations of functions and leveraging knowledge of their gradients. Despite their popularity, gradient-based methods do not guarantee the achievement of a global optimum and tend to be ineffective when dealing with a large number of system parameters. In the context of optimizing complex processes, the best choice is to use heuristic optimization methods [12], which are based on the principles of stochastic search and global optimization. The main drawback of these methods, when identifying a large number of system parameters, is their high demand for computational resources and slow execution speed. The integration of parallelization technologies can mitigate these limitations by distributing tasks across multiple processors or computing nodes. Clearly, the integration of cloud computing technologies and the implementation of proprietary methods and algorithms as a unified software package will provide an efficient digital tool for conducting comprehensive research into complex processes governed by polymerization mechanisms.

The goal of this work is to develop a cloud digital service that allows for comprehensive research of complex physicochemical processes occurring by the polymerization mechanism. The resulting digital product is a networked information system that can be used to conduct a series of computational experiments within the framework of empirical research and select optimal production organization modes.

2- Functional Purpose of the Cloud Service

Researching complex physicochemical processes implies the presence of a detailed mathematical description—a model that includes both the main equations describing the change in material balance for each reaction component and additional parameters affecting the process. When adapting the developed comprehensive methodology to polymer synthesis processes, we highlight the main types of tasks in the correct chronological sequence determining the functional purpose of the created digital product.

2-1- Restoration of the Kinetic Mechanism of Elementary Reactions

At the initial stage, from the primary physicochemical information in the form of a kinetic curve and the distribution of the product by molecular mass, it is necessary to solve the problem of restoring the kinetic scheme as a set of elementary stages and identifying the corresponding kinetic parameters [13]. If we are talking about homopolymerization processes, it is required to uniquely identify the picture of kinetic heterogeneity and determine the corresponding kinetic activity [14, 15] of each active center. Various approaches to assessing kinetic heterogeneity are based on the idea of representing the initial molecular weight distribution (MWD) of the polymer product as a superposition of n model distributions [16] characteristic of each type

$$q^{exp}(M) = p_1 K(\lambda_1, M) + p_2 K(\lambda_2, M) + \ldots + p_n K(\lambda_n, M), \quad (1)$$

where λ is the Frenkel statistical parameter, M is the molecular mass, $K(\lambda, M)$ is the expression defining one of the model distributions, p_i represents the fraction of each active center ($i = 1..n$). Figure 1 shows an example of visualizing such a decomposition for a catalytic system based on gadolinium chloride solvate [17].

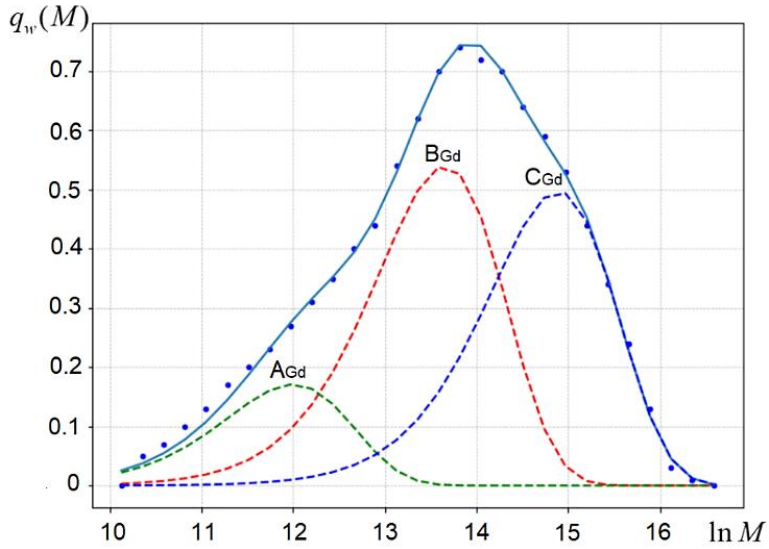

Figure 1. Decomposition of the initial MWD (solid line – experimental MWD curve, dashed line – distribution of the identified active centers)

The classical approach is based on the use of the regularization method proposed by Academician A.N. Tikhonov [18] and adapted for solving inverse problems of MWD formation [19]. An alternative simulation approach to solving the inverse problem, developed by the authors [20, 21], is based on the idea of reproducing various process scenarios and numerically evaluating the corresponding parameters.

2-2- Calculation of Physicochemical and Consumer Properties of the Product

The main molecular characteristics of the polymer product are evaluated based on solving the direct problem using both kinetic and statistical approaches to modeling for any representation from the set of formal kinetic schemes of elementary reactions.

The implementation of the kinetic approach to modeling is based on transforming the initial set of elementary reactions to form a system of ordinary differential equations. When describing polymer synthesis processes, the dimensionality of such systems becomes too high due to the rather large length of the formed macromolecules. In this case, statistical moments [1] of the molecular weight distribution m_j are introduced for analyzing the polymer product

$$m_j = \sum_{x=2}^{\infty} x^j M_x,\ \frac{dm_j}{dt} = \sum_{x=2}^{\infty} x^j \frac{dM_x}{dt}, \tag{2}$$

where M_x is the molar concentration of polymer chains of length x. The evaluation of the polymer product in this case is carried out by analyzing the averaged molecular characteristics [7], which include the number-average molecular mass $\overline{M_n}$, the weight-average molecular mass $\overline{M_w}$, and the z-average molecular mass $\overline{M_z}$. To estimate these, the knowledge of the initial moments is required:

$$\overline{M_n} = \frac{m_1}{m_0},\ \overline{M_w} = \frac{m_2}{m_1},\ \overline{M_z} = \frac{m_3}{m_2}. \tag{3}$$

The implementation of the statistical approach to modeling implies the constant fixation in the computer's dynamic memory of all variables determining the structure and molecular chain of each macromolecule. At the core of the statistical approach to modeling is an algorithm that allows forming possible solutions of systems using the Monte Carlo method [22] by organizing a series of trials.

Since for a reaction of the type $X_A + X_B \xrightarrow{\tilde{k}} X_{[A+B]}$the rate R_i is determined according to the law of mass action $R_i = \tilde{k}_i X_A X_B$ (where $\tilde{k}_i$ is the constant characterizing the rate of the given reaction, and $[X_A]$, $[X_B]$ are the molar concentrations of reactants X_A and X_B) it is always possible to calculate the probability of each reaction by finding the ratio of the rate of a given reaction to the sum of the rates of all reactions $p_i = R_i/(R_1 + R_2 + \ldots + R)$. Subsequently, according to the stochastic law, a reaction is chosen, and its modeling is carried out at the particle level. The number of molecules involved in the modeling determines the stability of the obtained results. The algorithm for implementing the kinetic and statistical approaches for modeling the processes of homo- and copolymerization is detailed in the works [23, 24].

2-3- Identification of Unknown Kinetic Parameters

In the presence of an existing mathematical model and sufficient computational resources, it is logical to use the "direct problem method" to solve inverse problems of chemical kinetics. This method involves calculating the molecular

weight distribution function or other molecular characteristics for the proposed kinetic scheme of the process and comparing the results with the corresponding experimental data. If a group of kinetic parameters k_i $(i = 1..p)$ affects the formation of a certain molecular characteristic $\overline{M}$, the task of identifying them can be represented as an optimization problem

$$H(k_1, k_2, .., k_p) = \sum_{i=1}^{n} [\overline{M}_i^{calc} - \overline{M}_i^{exp}]^2 \to min, \quad (4)$$

where $\bar{M}_i^{calc}, \bar{M}_i^{exp}$ are the calculated and experimental values of the molecular characteristic $\overline{M}$, respectively, for $i = 1..n$.

The Equation 4 can be solved using classical numerical methods of gradient descent [25] or heuristic optimization methods [26, 27]. The computational core of the information system includes software complexes for implementing all these algorithms.

2-4- Evaluation of Polymer Product Heterogeneity

The analysis of the heterogeneity of the resulting products in terms of molecular mass, size-composition, and composition is carried out within the framework of implementing the statistical modeling approach. The authors developed a method for numerical processing of polymer macromolecules, based on the digital simulation of their fractionation procedure [28].

In particular, for assessing the MWD of homopolymerization products, each modeled macromolecule is analyzed, its mass is calculated each time, and the resulting values are divided into groups (or fractions) with a given fractionation step. For each formed fraction, the sum of the fraction and its mass share are calculated, which ultimately allows reproducing the MWD curve of the product from a chaotic set of data (Figure 2).

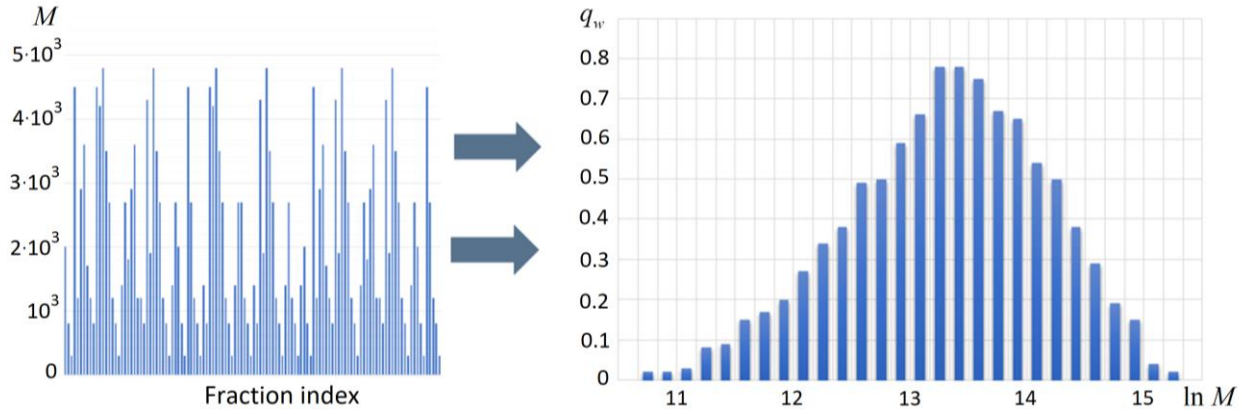

Figure 2. Methodology for evaluating the molecular weight distribution of the product as a result of digital fractionation of macromolecules

The methodology for evaluating the size-composition distribution [29] for copolymers extends the idea of reproducing the MWD. The main difference is that when selecting macromolecules, it is necessary to check their compliance with the specified composition before performing further fractional division.

2-5- Determining the Optimal Composition of the Initial Reaction Mixture

Within the framework of the kinetic approach implementation, the mathematical model of the process represents a system of ordinary differential equations

$$\frac{dX_i}{dt} = F_i(t, X_i(t)), i = 1..n \quad (5)$$

with initial conditions $X_i(0) = X_i^0$ for all $i = 1..n$, where $X(t)$ – the vector determining the concentrations of all initial reaction components at the initial time $t \in [0, t_{end}]$. To determine the optimal composition of the initial reaction mixture, it is necessary to find the vector of initial concentrations $X^*(0) = (x_1^*(0), x_2^*(0), \ldots, x_n^*(0))$, for which, at the final modeling time t_{end}, the system reaches the target state $\tilde{X}$ by the m system parameters. The optimization criterion is considered a functional

$$G(X^*(0)) = \sum_{i=1}^{m} \left| X_i(t_{end}) - \tilde{X}_i \right| \to min, \ m \le n. \quad (6)$$

Heuristic optimization methods [27] are used to solve optimization problems (6), among which genetic algorithms [30-33] based on the mechanism of creating a population of potential solutions using probabilistic laws are predominant.

Based on the presented calculation methods, corresponding algorithms have been developed for each type of task, and their software implementation has been completed. Although each algorithm incorporates standardized calculation methods applicable to a wide range of physicochemical processes governed by different mechanisms, the core computational logic has been adapted to the specifics of polymerization processes. In particular, within the framework of the kinetic approach, implicit schemes of numerical methods (the fourth-order Adams-Moulton method) are used to predict the properties of the final product. To handle the vast number of operations within the statistical approach, the mechanism of CUDA core utilization of the GPU and cloud network resources has been employed. The tasks of experimental design and determining the optimal initial composition of the reaction mixture for polymer synthesis processes are solved using heuristic optimization methods, which ensure a solution is reached within a finite number of iterations. The graphical model illustrating the main methodological approach to investigating polymer synthesis processes, utilizing the previously described methods and approaches, is presented in Figure 3.

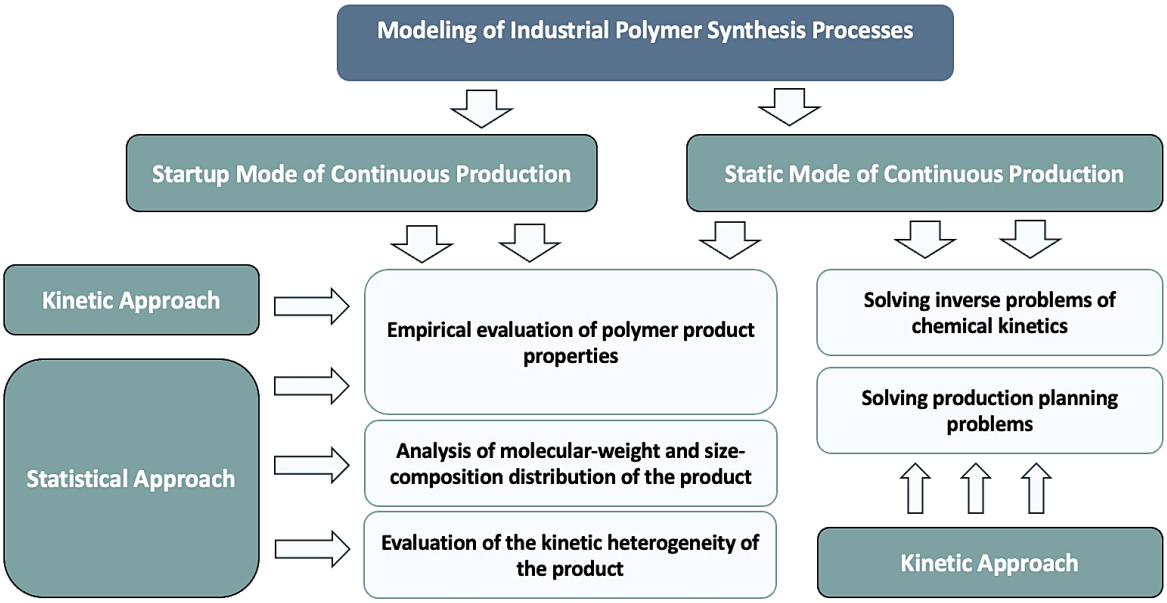

Figure 3. The graphical model defines the methodological approach to the investigation of polymer synthesis processes

3- Organizational Structure of the Information System

The network interaction system of the developed cloud service aimed at comprehensive research of complex physicochemical processes has an extended network architecture [30-34] represented by three levels.

3-1- The Client Part

The client part is the first level of the information system, where the main interaction with users occurs, allowing the selection of the type of task to be solved and all necessary initial conditions. Since the information system is oriented towards multi-user mode, the functionality of this level includes managing all computational resources (CPU cores, CUDA GPUs, memory volume, etc.). For organizing this work, significant computational resources are not required, and any device falling under the definition of a "thin client" can handle the tasks.

The client part also provides access to the calculation results in both graphical and tabular forms, preserving the history of all performed calculations in the user's personal account. For general convenience, the client part is presented as a web interface shell written using the Blazor C# web framework [35], supporting cross-platform work and allowing creating client-side application logic in C#, utilizing all advantages of the .NET ecosystem. Blazor, as part of the .NET ecosystem, offers the ability to use a single programming language — C# — both on the client and server sides, which significantly simplifies development and reduces the likelihood of errors related to using different programming languages at various levels of the architecture. Additionally, Blazor provides a high degree of integration with cloud services, making it an ideal choice for projects focused on cloud deployment and operation. This capability allows for easy scaling of the application depending on the load and ensures reliable resource management in a cloud environment. Blazor's performance advantages are particularly evident in scenarios where server-side computations and data security are critical.

The visualization of the obtained task solution results is handled by the "plotly.js" library, which allows creating interactive graphs and visualizing data directly in the browser. Unlike other tools, the "plotly.js" library efficiently processes and visualizes large data sets, which is particularly relevant when analyzing the formed polymer macromolecules.

3-2- The Data Storage System

The data storage system is the second level of the information system, ensuring the storage of computational experiment results and all reference information determining the main physicochemical data. Within the framework of implementing the simulation approach to modeling, the data volume can be extremely large, so this level is physically separated from the rest of the architecture and located on a separate server.

The work of this level is organized under the control of the MongoDB [36] database management system (DBMS). Unlike other solutions, this DBMS initially supports the sharding function [37], allowing horizontal scaling and managing large volumes of data distributed across multiple servers/clusters. At the same time, for both the end user and the developer, these tables will be perceived as a unified database. In the context of researching physicochemical processes, this is especially relevant since the database structure and its size may exceed acceptable limits. These issues become particularly critical within the framework of simulation-based modeling, where the success of computations depends on the volume of data being processed. Additionally, MongoDB supports the replication function, allowing the creation and maintenance of data copies on multiple servers (replicas) to ensure fault tolerance, increase data availability, and improve performance. The use of this feature and the organization of corresponding duplication rules for changes simplify the operation of a hybrid cloud, where part of the computations is performed locally and part remotely. This is particularly relevant when organizing the logic of cloud computing execution.

3-3- The Computational Organization System

The computational organization system is the third level of the information system, responsible for organizing all calculations using remote network resources. The server on which this level is located has the highest technical requirements, the volume of which determines the speed and efficiency in solving tasks.

All previously developed methods and algorithms by the authors constitute the main array of computational modules and libraries written in different programming languages and comprising the computational core of this information system.

The integrated management program is responsible for launching these computational programs and libraries in remote mode [38]. Resource distribution is carried out using Docker containerization technology [39-41], representing software virtualization at the operating system level managed by its kernel. Unlike virtual machines, containers do not require a separate operating system and instead use the host's operating system kernel, making them more efficient. Docker containers allow easy system scaling by increasing computational power through the addition of new application instances. Additionally, Docker simplifies dependency management, facilitating the deployment and updating of complex systems. The main challenges of Docker containerization are related to the fact that containers typically do not retain state, necessitating the use of external storage for data. The conceptual scheme of interaction between all three levels of the information system is presented in Figure 4.

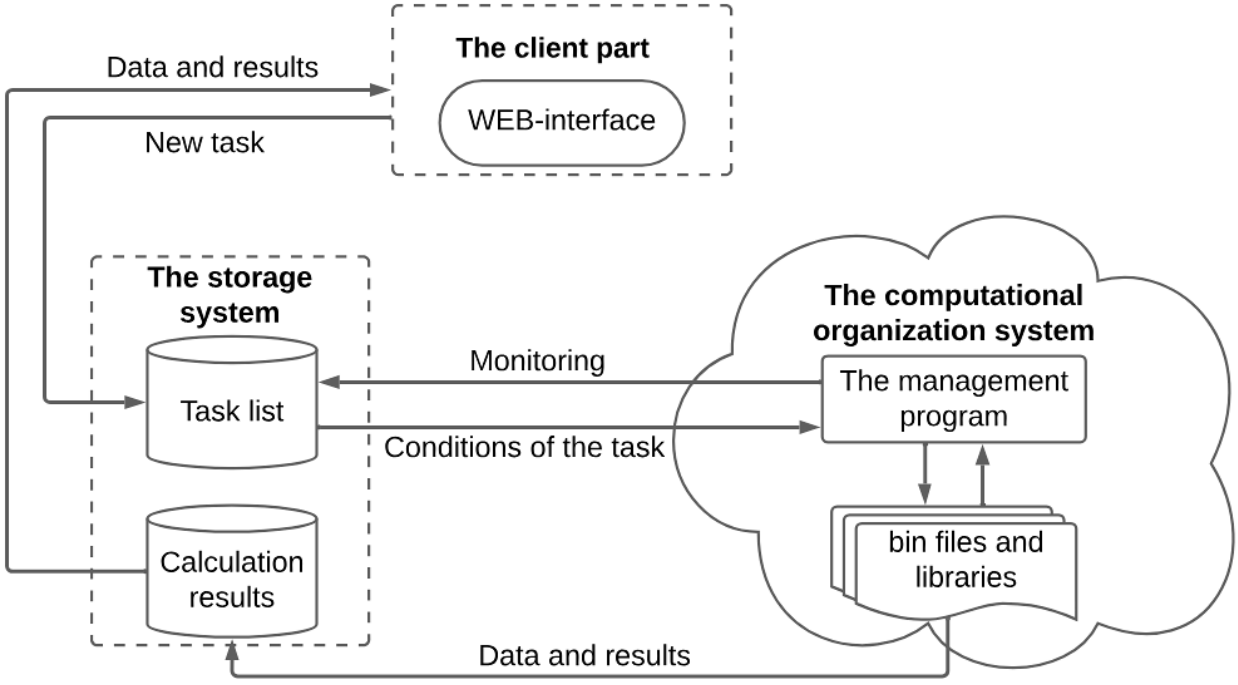

Figure 4. Conceptual scheme of the remote computation system organization

The organization of direct network communication using standard GET and POST requests is not feasible [41] due to the periodic load on the central server. Therefore, to ensure the continuous operation of all presented layers, the developed service implements an algorithm for contactless network interaction. The core of the algorithm is based on designing and utilizing a specialized task scheduler that uses a dedicated table in the central database.

The table's structure is organized in such a way as to contain data on the status of each task, from its creation to the completion of all calculations. The table structure is shown in Table 1.

Table 1. Structure of the table for organizing network interaction

Field Name	*Description*	*Data Type*
id_task	Task identifier	Numeric
date_task	Task creation date and time	Date/Time
author_task	Task author identifier	Numeric
status	Task status	Text
type_of_task	Task type	Text
priority	Priority	Numeric
parameters	Initial conditions	Reference
bin_file	Execution program	Text
results	Execution results	Text

The operation of the cloud service can be outlined in the following chronological order:

When a new task is created, an entry is automatically generated in the table, where it is assigned a unique identifier. The "status" field in the table reflects the status of the task as "not started."

The control program, which operates at the computation management system level, periodically checks the table. If a new task is detected and free computational resources are available, the control program, based on the type of task and its assigned priority, invokes the corresponding executable file for execution and changes the task status to "in progress."

During the task execution, the control program periodically checks the task scheduler to identify the task based on its unique identifier. Since the task might not be completed and could fail with an unexpected error (due to incorrect formulation or inability to compute using the chosen method), the control program additionally verifies the task completion status. If the task is successfully completed, the status is updated to "calculation finished."

The module responsible for the client-side also periodically checks the status updates of tasks. Once the calculation for the current task is fully completed, a link to all the execution results is generated.

Since it is almost impossible to structure different types of tasks under a single format, the principle of data transmission via typed input (input.) and output (output.) files are used for interaction between the interface part and the computational organization system.

The input.dat file is used to transfer data from the interface part to the calculator, and the output.dat file – to transfer calculation results back to the interface part. The data flow diagram (DFD) between the interface part and the computational organization system is presented on Figure 5.

The management program's functions include periodically monitoring the completion status of previously set tasks. This control is necessary for constant accounting and operational division of free computational resources. All calculation results are recorded in the respective working tables of the central database, accessible from the client part of the information system.

The developed digital product supports the integration of new computational modules from third-party developers. Currently, the system supports the integration of software modules written in C, C++, Python, and Java. To address the challenge of forming the interface and creating corresponding dialog windows, a third-party computational module is integrated into the system along with a configuration file (*.ini file). Based on the contents of this file, the system automatically generates the interface elements. The dynamic rendering of input parameters for the dialog window, which defines all the initial task parameters, is carried out each time the configuration *.ini file is detected in the directory of the executable program.

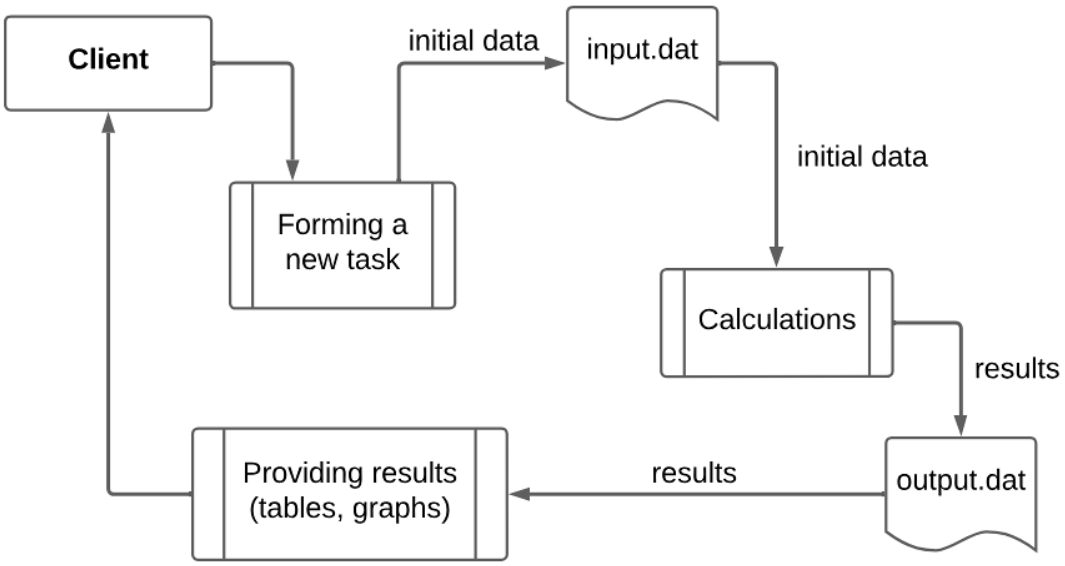

Figure 5. DFD diagram of data flows between the interface part and the computational organization system

4- Computation Organization

To start working with the cloud service, you need to go to the appropriate network address to access the user's personal account, where the history of previously conducted calculations is reflected by default, each of which has a unique identifier— the "id" field (Figure 6).

Id	Name	BinPath	Description	Actions
70ba577f98531c47fb82756f	Polymerization of isoprene	2typeAC_polymer.py	2typeAC_polymer without DIBAH	EDIT
610518a76605101254312a66	Copolymerization of butadiene and styrene	Copol_period_kin.cpp	Copolymerization (periodic mode) kinetic method	EDIT

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Figure 6. Calculation history in the user's personal account

If the calculation has not yet been initiated by the user, there is only the possibility to edit the initial conditions in the "actions" field. If the task has already been solved, corresponding menu items appear allowing you to view both all initial task parameters ("view params") and the solution results in graphical form ("show result").

4-1- Comprehensive Study of the Homopolymerization Process

We use the information system's functionality to solve the task of restoring the nature of kinetic heterogeneity on the example of 1,4-cis-polyisoprene production in the presence of a titanium-containing catalyst. The suspension was obtained at -10°C by mixing toluene solutions of $TiCl_4$ (catalyst) with $Al(i-C_4H_9)_3$ (co-catalyst), the p-electron donor additive diphenyl oxide (DPO), and the σ-electron donor additive piperilene (Pip) in a ratio of $TiCl_4/Al(i-C_4H_9)_3$/Pip/DPO = 1 mol/1 mol/0.2 mol/0.15 mol. The conditions for preparing the catalyst and obtaining the polymer product are described in detail by Nasyrov et al. [42].

The obtained polyisoprene was studied by gel permeation chromatography using the "Alliance GPCV-2000" liquid chromatograph (Waters) equipped with refractometric and viscometric detectors. The results of the analysis in the discrete representation of the initial MWD curve are presented on Table 2. The width of the molecular weight distribution of the product is represented by the polydispersity value M_w/M_n= 2.56.

Table 2. Discrete representation of experimental results

lgM	q_i	lgM	q_i	lgM	q_i
4.2	0	5.2	0.34	6.2	0.67
4.4	0.03	5.4	0.44	6.4	0.5
4.6	0.08	5.6	0.54	6.6	0.27
4.8	0.15	5.8	0.71	6.8	0.07
5.0	0.25	6.0	0.78	7.0	0.01

The input of initial information is performed via an uploadable typed file, in accordance with the format in which the data needs to be presented in two columns: the first column - lgM, the second column - q_i values, defining the MWD curve. The file will look like this:

```
4.2 0
4.4 0.03
…
6.8 0.07
7.0 0.01
```

After uploading the file, it is necessary to specify the error magnitude of the experimental data, choose the method for solving the inverse problem, and launch the software module. The computational core of the information system contains two executable files for organizing the calculations: method_regul.py (A.N. Tikhonov's regularization method) and imitation_method.py (imitation approach), both written in Python. During the functional testing of the information system, the imitation approach was chosen for solving the inverse problem, and the graphical results are presented in Figure 7 as curves characterizing the distribution for each active center. Thus, the computations demonstrate that for the given catalytic system, two types of active centers can be identified — type A and type B, with characteristic average molecular masses for each type: lnM=11.5 (A) and lnM =13.4 (B). The content of type A active centers in the catalyst is 8.1%, while type B accounts for 91.9%. The obtained numerical assessment of kinetic heterogeneity aligns with previously reported results [43], and the applied approach shows higher accuracy without the need for additional analysis of the active center distribution curve.

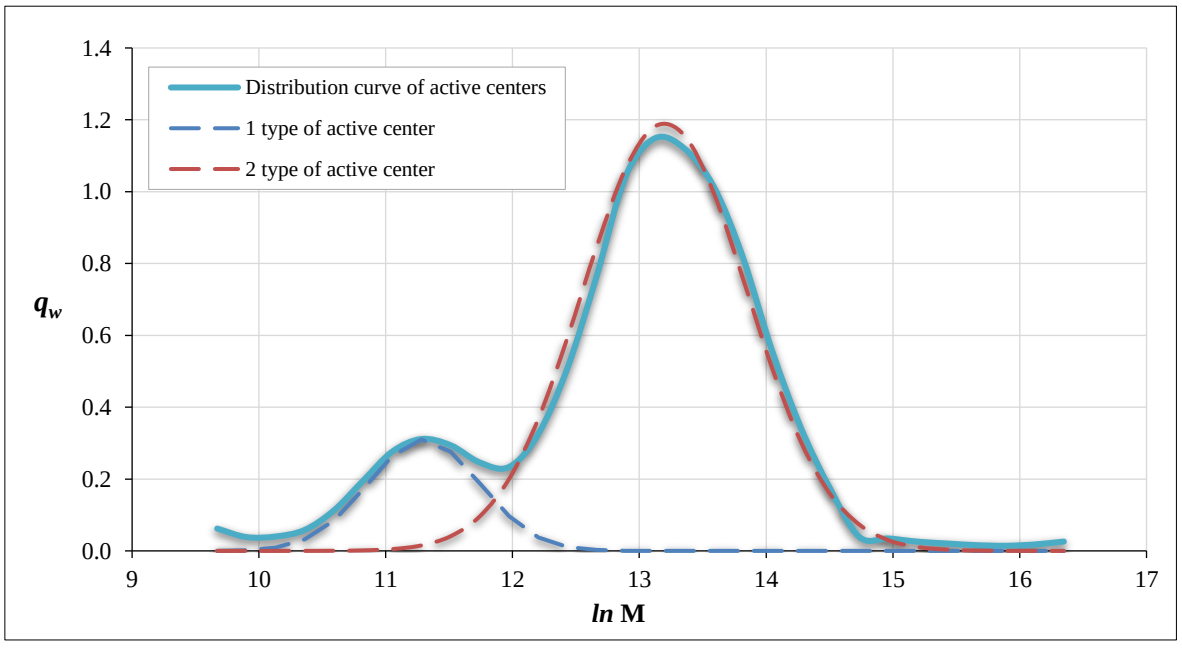

Figure 7. Results of solving the inverse problem of MWD formation

On this same page, there is an option to download the program execution results as a text file. With information on the dynamics of the active centers, it is possible to set and successfully solve the tasks of calculating the physicochemical and consumer properties of the product depending on the composition of the initial reaction mixture. To do this, a new task needs to be created, and the executable file 2typeAC_polymer.py should be selected as the main method of solution. In the dialog box that appears (Figure 8), it is necessary to set the main technological parameters of the process, including the number of active center types, the modeling time, the batch composition, and the kinetic parameters characterizing the rates of individual reactions.

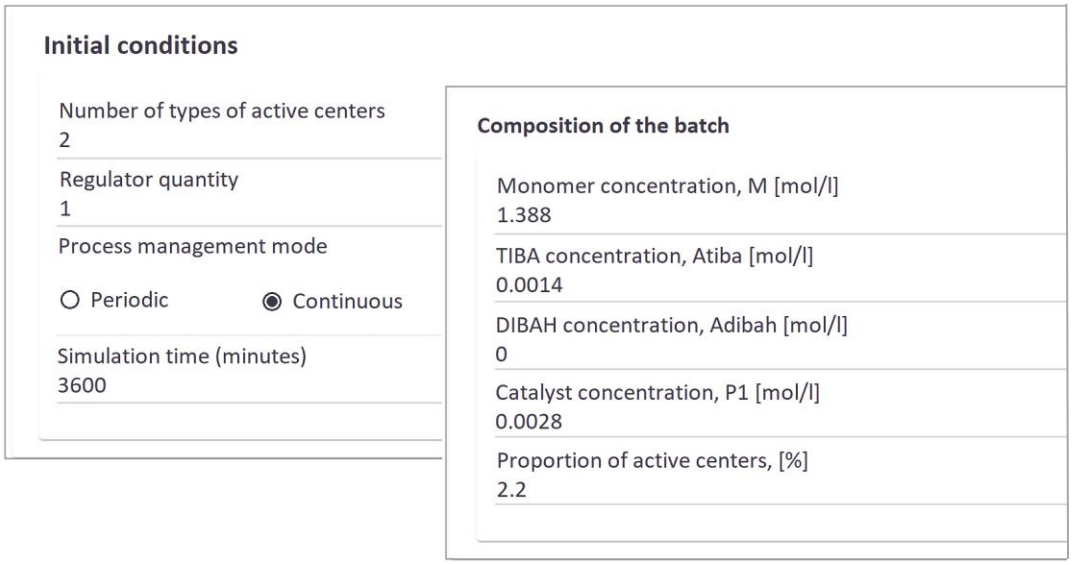

Figure 8. Determination of the main technological parameters of production

After obtaining a unique identifier for the specified technological conditions, the task will be solved in order of queue and availability of free computational resources. The "show result" menu item allows you to obtain the results both in graphical form (Figure 9) and in tabular representation. In the same window, there is an option to configure the display and visualization parameters of the results. In particular, the presented graph reflects the dependence of the polydispersity of the polymer product, determined by the ratio M_w/M_n. The points on the graph represent the results of a previously conducted laboratory experiment, and their consistency with the calculated data allows for the evaluation of the accuracy of the obtained results.

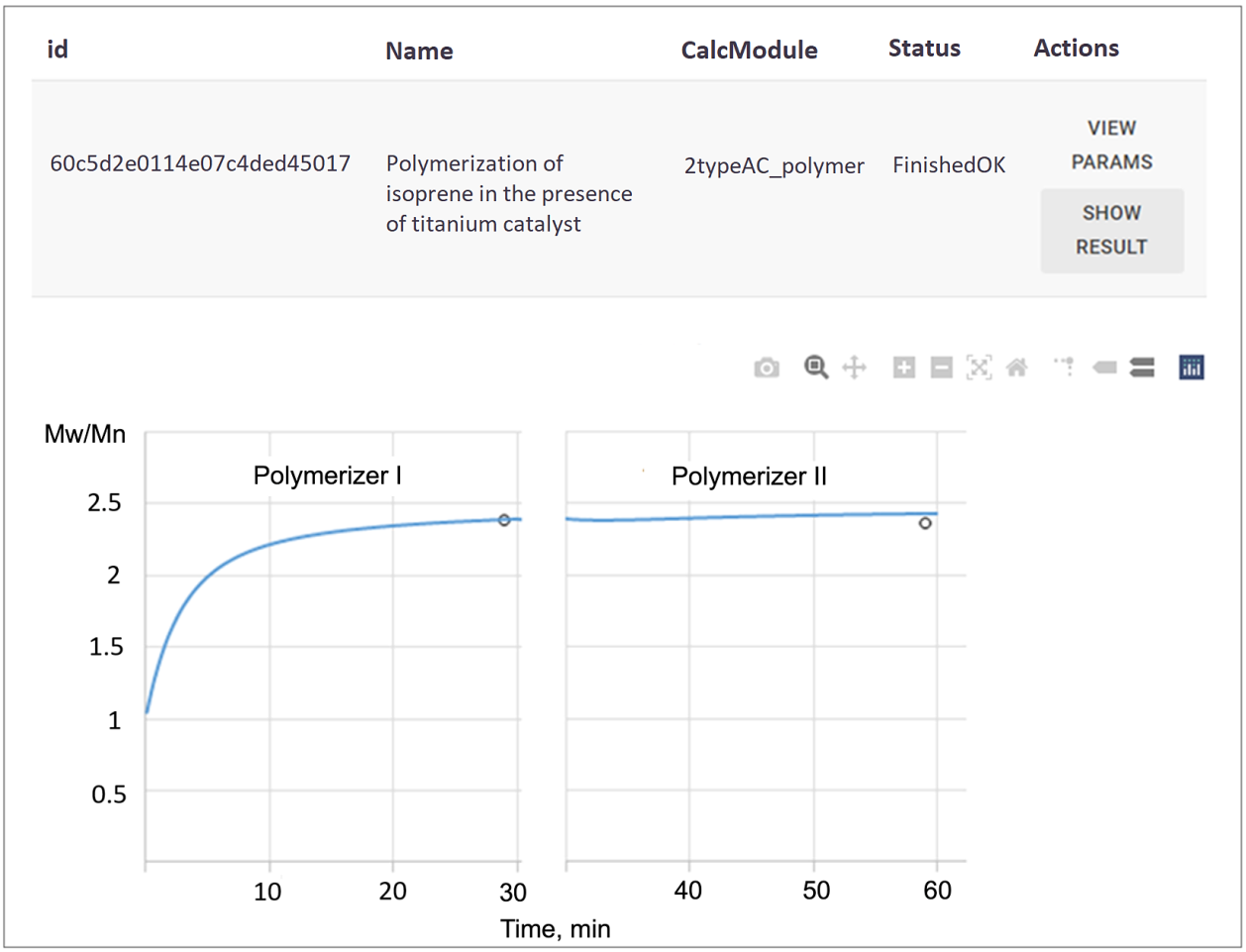

Figure 9. Presentation of task solution results

The advantages of the developed digital service include the ability to utilize cloud network resources for implementing a simulation-based approach to modeling and assessing the detailed properties of the product at the macromolecular level. In particular, Figure 10 presents the results of the software module focused on evaluating the molecular weight distribution of the polymerization product for each active center, and the obtained results are consistent with the initial molecular weight distribution.

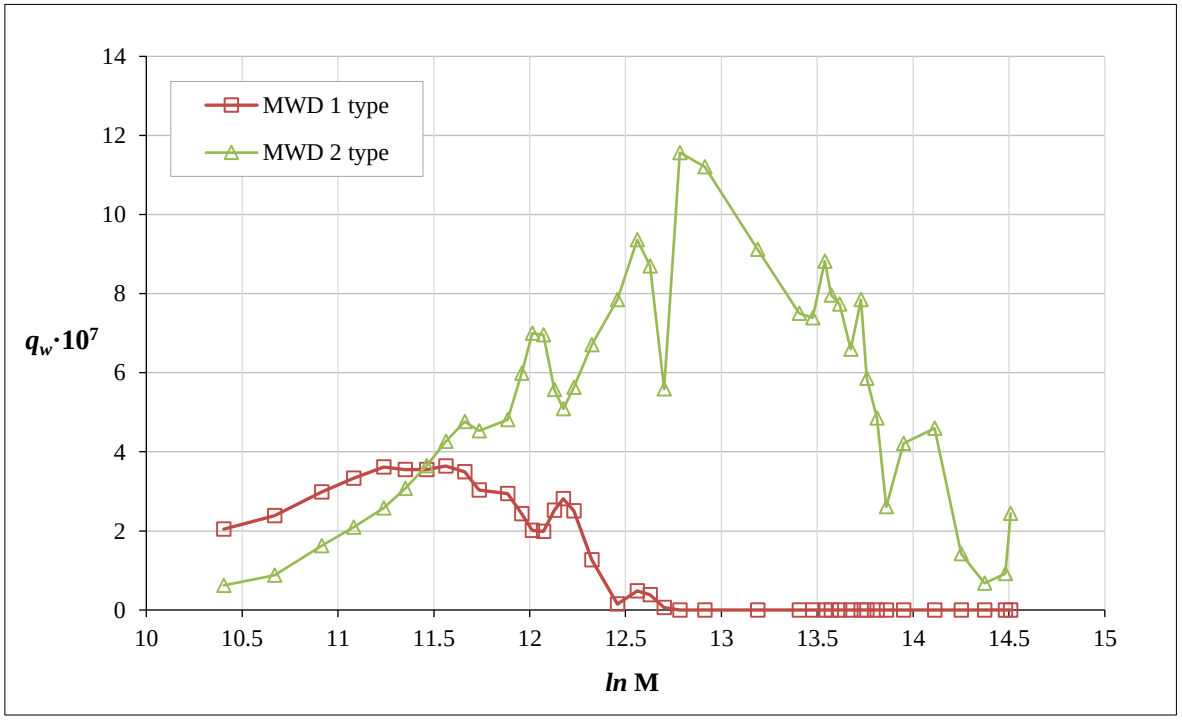

Figure 10. Molecular weight distribution of the isoprene polymerization product in the presence of a titanium-containing catalytic system (dashed line – active center type 1, solid line – active center type 2)

4-2- Evaluation of Compositional Heterogeneity of the Copolymerization Product

To test the capabilities of the developed cloud service, the most computationally challenging task was addressed — the evaluation of the compositional heterogeneity of the butadiene-styrene copolymerization product. According to production conditions, the copolymerization process takes place in a cascade of 12 continuous stirred-tank reactors with a monomer mass feed rate of 3.5 t/h. The process is initiated using pinane hydroperoxide at a dosage of 0.054 parts by mass per 100 parts by mass of monomers. The hydrocarbon phase is prepared by continuously mixing butadiene and styrene in a mass ratio of 70/30. The mass ratio of water to monomers is 220/100. Molecular weight regulation is carried out by adding a 5% solution of tert-dodecyl mercaptan (0.125 parts by mass per 100 parts by mass of monomers) at the beginning of the process, followed by the addition of a 1% emulsion at 0.027 parts by mass per 100 parts by mass of monomers into the third and sixth polymerizers. The kinetic mechanism and the model description for the specified experimental conditions are detailed in Miftakhov et al. [29].

In accordance with the specified conditions, the minimum statistical ensemble with a total volume of 10^6 molecules was calculated. During a series of computational trials simulating the formation of macromolecules until reaching a final monomer conversion of 70%, an evaluation of the resulting size-composition distribution curves was conducted (Figure 11). The mass content of butadiene in the modeled macromolecules was set in the range of 76 to 80%, as the most probable based on the given initial monomer ratio.

A visual assessment of the curves shows that the resulting product is heterogeneous and contains copolymers of varying compositions. The most probable composition of the copolymer at the specified conversion corresponds to a butadiene content of 76% (by mass) (curve 1), which aligns with the stated parameters of continuous industrial production. The lowest proportion of high-molecular-weight copolymers is observed when the butadiene-to-styrene ratio in the copolymerization product is 80:20. The obtained results are consistent with the previous evaluation from Miftakhov et al. [29] but demonstrate higher accuracy in reproduction.

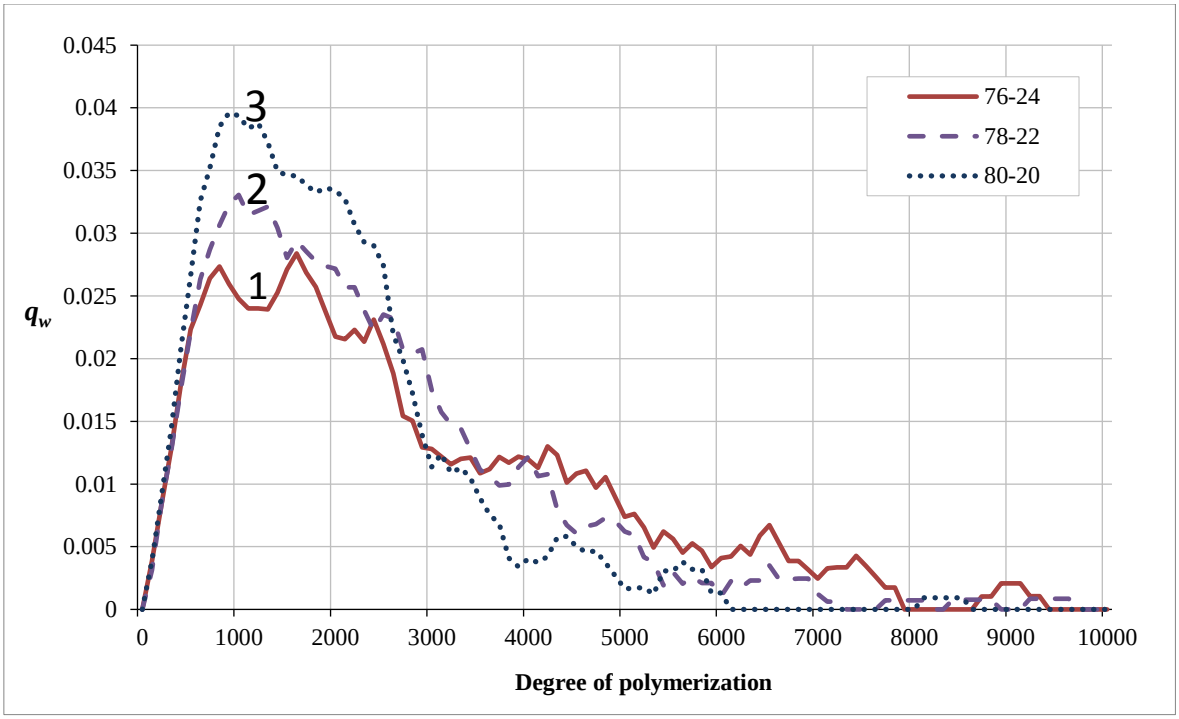

Figure 11. The size-composition distribution of macromolecules for different butadiene-to-styrene mass ratios in the copolymerization product at 70% conversion (curve 1– 76%: 24% (solid line); 2 – 78%: 22% (dashed); 3 – 80%: 20%)

It is evident that the superposition of the size-composition distribution curves, constructed for different copolymer compositions, represents the molecular weight distribution of the final product. It is important to note that the developed tools for evaluating the compositional heterogeneity of the product, integrated as software modules in the cloud service, are universal and can be applied to other copolymerization processes, where the kinetic mechanism and model description are known.

5- Conclusion

Thus, a comprehensive study of complex processes, which necessitates the processing of large streams of physicochemical data, requires the use of non-trivial computational schemes capable of handling the given tasks. In this regard, all previously developed proprietary models, methods, and algorithms were adapted for polymer synthesis processes and integrated into a cloud-based web service characterized by a three-tier network architecture, providing innovative principles for performing computations. The computational core of this system includes software modules and algorithms that have previously been successfully tested in real production processes. The core algorithms for organizing calculations are based on kinetic and statistical modeling approaches. The developed digital product enables a sequential methodological approach for conducting a comprehensive study of the declared processes, including various types of direct and inverse problem-solving in chemical kinetics. The developed network interaction algorithm allows the use of this service in a 24-hour mode for both standard empirical assessments and the selection of optimal continuous production scenarios. Despite the extensive list of built-in libraries for organizing calculations, this system is open to third-party developers. Thanks to the mechanisms of dynamic rendering, the web interface part of this service does not require additional configuration and is updated every time depending on the selected module for task solving. Computational experiments conducted for homo- and copolymerization processes have demonstrated the system's efficiency in solving various types of problems and its high accuracy in detailed assessments of the physicochemical properties of the resulting product.

6- Declarations

6-1- Author Contributions

Conceptualization, E.M. and S.M.; methodology, E.M. and A.K.; software, E.M. and S.M.; validation, A.A. and A.K.; formal analysis, E.M. and A.A.; investigation, S.M. and A.K. All authors have read and agreed to the published version of the manuscript.

6-2- Data Availability Statement

The data presented in this study are available in the article.

6-3- Funding

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6-4- Institutional Review Board Statement

Not applicable.

6-5- Informed Consent Statement

Not applicable.

6-6- Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this manuscript. In addition, the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, and redundancies have been completely observed by the authors.

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