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Developing Methods and Algorithms for Cloud Computing Management Systems in Industrial Polymer Synthesis Processes

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Abstract

To date, the resources and computational capacity of companies have been insufficient to evaluate the technological properties of emerging products based on mathematical modelling tools. Often, several calculations have to be performed with different initial data. A remote computing system using a high-performance cluster can overcome this challenge. This study aims to develop unified methods and algorithms for a remote computing management system for modelling polymer synthesis processes at a continuous production scale. The mathematical description of the problem-solving algorithms is based on a kinetic approach to process investigation. A conceptual scheme for the proposed service can be built as a multi-level architecture with distributed layers for data storage and computation. This approach provides the basis for a unified database of laboratory and computational experiments to address and solve promising problems in the use of neural network technologies in chemical kinetics. The methods and algorithms embedded in the system eliminate the need for model description. The operation of the system was tested by simulating the simultaneous statement and computation of 15 to 30 tasks for an industrially significant polymer production process. Analysis of the time required showed a nearly 10-fold increase in the rate of operation when managing a set of similar tasks. The analysis shows that the described formulation and solution of problems is more time-efficient and provides better production modes.

Keywords:

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

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1- Introduction

Recent developments of highly efficient technologies in the chemical and technological industries have increased the need for new energy-saving chemical and technological processes and systems to obtain production products with specific properties. A particular concern is modelling programmes and algorithms that evaluate the technological properties of products and serve as a tool for the selection of optimal production conditions [1]. The mathematical description of the process using basic mathematical models of physical and chemical hydrodynamics and chemical (macro) kinetics [2], as well as the insufficient resource and computer base of a company, pose a challenge. A single solution to a direct problem of predicting product properties as a function of initial cargo and ordered technological aspects of production requires enormous computational resources. It is almost certain that the search for optimal production modes requires multiple solutions to a direct problem and consequently demonstrates the impossibility of computing such problems with standard resources in a reasonable time.

A high-performance cluster that manages all computational experiments can solve the problem of insufficient computational resources. Since these computations need to be performed by several people at the same time, a possible

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solution is to assign all the computational logic to a remote server and give clients access to the network resources. This study proposes a network calculation management [3-7] for the industrial synthesis of polymer products. The concept of computation management can be applied to a wider area of the chemical industry. In previous research work, the authors of the present study have initiated the development of local software products that enable the private exploration of physicochemical processes. A number of them are registered in the Federal Service for Intellectual Property [8, 9]. However, they are not capable of solving problems different from those originally stated. Moreover, these software products do not support multi-user and remote operations.

This study aims to develop unified methods and algorithms for a remote computing management system for modelling polymer synthesis processes at a continuous production scale. It can solve multiple client tasks simultaneously, using computing resources according to the problem and priority.

1-1-Mathematical Description of the Industrial Synthesis of Polymers

Traditionally, polymer products production is described in terms of the continuous process in a cascade of perfectly mixed reactors [10]. Figure 1 presents a scheme for producing cis-1,4-polyisoprene obtained by isoprene polymerization in titanium and neodymium catalytic systems [11]. After loading the entire reaction mixture into the first reactor of the cascade, there is a series of sequential reactions.



Figure 1. Scheme of continuous polyisoprene production.

In particular, the kinetic mechanism [12] of polyisoprene production in the titanium-based catalytic system causes successive reactions initiating active centers, the polymer chain propagation and its termination by transfer mechanisms, spontaneous breakage, and possible chain reactions. The most complete description is as follows:

- 1. The polymer chain propagation by attaching a monomer molecule $P_i^j + M \xrightarrow{k_p^j} P_{i+1}^j$
- 2. Polymer chain transfer to monomer molecules $P_i^j + M \xrightarrow{k_m^j} Q_i + P_1^j$
- 3. Chain transfer to the regulator (aluminium organic compound) $P_i^j + A \xrightarrow{k_a^j} Q_i + P_1^j$
- 4. Possible decay of active centers $P_i^j \xrightarrow{k_d^j} Q_i$

5. Transition of active centers to each other:

$$\begin{array}{c}
P_i^1 & \xrightarrow{k_c^{12}} & P_i^2, \\
P_i^2 & \xrightarrow{k_c^{21}} & P_i^1,
\end{array}$$

 $k_n^j, k_c^{jk}, k_a^j, k_m^j, k_d^j$ where *M* is monomer *A* AC concentration, j = 1, 2 characterizes the type of the active center, P_i^j active ("growing") polymer chain of the length *i* on *j* the type of active centers; Q_i inactive ("dead") polymer chain of the length *i*, $k_n^j, k_c^{jk}, k_a^j, k_m^j, k_d^j$ – constants describing the chain propagation rate, the transition of active centers in each other, and chain transfer to an aluminium organic compound, the monomer and the possible decay of active centers, respectively. Then, a system of differential equations is worked out based on the mass action law. They represent the change in the material balance for each component of the reaction [2]. Since the length of polymer chains can reach hundreds of thousands of molecules, the resulting system of differential equations is characterized by a high dimension (10⁵-10⁶).

$$\begin{cases} \frac{dM}{dt} = -M\left(\sum_{i=0}^{\infty} P_{i}^{1}\left(k_{p}^{1}+k_{m}^{1}\right)+\sum_{i=0}^{\infty} P_{i}^{2}\left(k_{p}^{2}+k_{m}^{2}\right)\right),\\ \frac{dA}{dt} = -A\left(k_{a}^{1}\sum_{i=0}^{\infty} P_{i}^{1}+k_{a}^{2}\sum_{i=0}^{\infty} P_{i}^{2}\right),\\ \frac{dP_{1}^{1}}{dt} = -k_{p}^{1}MP_{1}^{1}+\left(k_{m}^{1}M+k_{a}^{1}A\right)\sum_{i=2}^{\infty} P_{i}^{1}-k_{d}^{1}P_{1}^{1}+k_{c}^{21}P_{1}^{2}-k_{c}^{12}P_{1}^{1},\\ \frac{dP_{1}^{2}}{dt} = -k_{p}^{2}MP_{1}^{2}+\left(k_{m}^{2}M+k_{a}^{2}A\right)\sum_{i=2}^{\infty} P_{i}^{2}-k_{d}^{2}P_{1}^{2}+k_{c}^{12}P_{1}^{1}-k_{c}^{21}P_{1}^{2},\\ \frac{dQ_{1}^{1}}{dt} = k_{m}^{1}MP_{1}^{1}+k_{a}^{1}AP_{1}^{1}+k_{d}^{1}P_{1}^{1},\\ \frac{dQ_{1}^{2}}{dt} = k_{m}^{2}MP_{1}^{2}+k_{a}^{2}AP_{1}^{2}+k_{d}^{2}P_{1}^{2},\\ \frac{dP_{1}^{i}}{dt} = k_{p}^{1}M\left(P_{i-1}^{1}-P_{i}^{1}\right)-k_{m}^{1}MP_{i}^{1}-k_{a}^{1}AP_{i}^{1}-k_{c}^{12}P_{i}^{1}+k_{c}^{21}P_{i}^{2},\\ \frac{dP_{1}^{2}}{dt} = k_{p}^{2}M\left(P_{i-1}^{2}-P_{i}^{2}\right)-k_{m}^{2}MP_{i}^{2}-k_{a}^{2}AP_{i}^{2}-k_{d}^{2}P_{i}^{2}+k_{c}^{12}P_{i}^{1}-k_{c}^{21}P_{i}^{2},\\ \frac{dP_{1}^{2}}{dt} = k_{p}^{2}M\left(P_{i-1}^{2}-P_{i}^{2}\right)-k_{m}^{2}MP_{i}^{2}-k_{d}^{2}AP_{i}^{2}+k_{c}^{2}P_{i}^{1}-k_{c}^{21}P_{i}^{2},\\ \frac{dQ_{1}^{2}}{dt} = k_{m}^{1}MP_{i}^{1}+k_{m}^{1}AP_{i}^{1}+k_{d}^{1}P_{i}^{1},\\ \frac{dQ_{1}^{2}}{dt} = k_{m}^{1}MP_{i}^{1}+k_{m}^{1}AP_{i}^{1}+k_{d}^{1}P_{i}^{1},\\ \frac{dQ_{1}^{2}}{dt} = k_{m}^{2}MP_{i}^{2}+k_{m}^{2}AP_{i}^{2}+k_{d}^{2}P_{i}^{2}. \end{cases}$$

To reduce the system of equations to a finite form, the concepts of active and inactive circuit moments are introduced: $\mu_j^k = \sum_{i=2}^{+\infty} i^j P_i^k, \quad \eta_j^k = \sum_{i=2}^{+\infty} i^j Q_i^k, \quad (2)$

which enables the description of the process for predicting the averaged molecular characteristics according to the equations [2]:

$$M_{n} = m_{0} \frac{\mu_{1}^{1} + \mu_{1}^{2} + \eta_{1}^{1} + \eta_{1}^{2}}{\mu_{0}^{1} + \mu_{0}^{2} + \eta_{0}^{1} + \eta_{0}^{2}},$$

$$M_{w} = m_{0} \frac{\mu_{2}^{1} + \mu_{2}^{2} + \eta_{2}^{1} + \eta_{2}^{2}}{\mu_{1}^{1} + \mu_{1}^{2} + \eta_{1}^{1} + \eta_{1}^{2}},$$
(3)

where M_n and M_w are the average calculated and average mass molecular weight, respectively, and m_0 is the molar цушпре of the initial monomer.

In its final representation, the mathematical model of the process is represented by a system of differential equations of finite dimension. Implicit schemes of numerical methods for finding differential equations can be used to solve the system to predict the molecular and consumer parameters of a polymer product. Since industrial scale production is assumed to be continuous flow, it is necessary to capture hydrodynamic laws to describe the process in the reactor cascade. If it is assumed that the technological conditions in production do not change over a long period of time and that within a single cascade reactor there are no changes in the product properties and concentrations of the initial substances, the technological process can be considered stationary (static). Based on this assumption, the mathematical description of the process can be extended by recurrent relations as follows:

$$\frac{\left(\bar{Y}^{(k-1)} - \bar{Y}^{(k)}\right)}{\theta^{(k)}} + \bar{R}_{y}^{(k)} = 0,$$
(4)

where $\theta^{(k)}$ stands for the residence time of the reaction mixture in *k*-the cascade reactor and the form $\overline{R}_{y}^{(k)}$ is determined by the adopted kinetic module, vector *Y* is determined by the dimension of the system of Equations 1 and therefore $Y = (M, A_{TIBA}, A_{DIBAG}, P_1, Q_1, \mu_0, \eta_0, \mu_1, \eta_1, \mu_2, \eta_2)$. It should be noted that the described modification makes it possible to switch from a system of differential equations to a system of nonlinear equations, the numerical solution of which requires less computational resources, but the number of such systems directly depends on the number of reactors of the continuous production cascade.

2- Data and Methodology

2-2- A Conceptual Scheme of the Remote Computing Management System

The network interaction in the information system for managing remote computing is represented by a three-tier architecture [13-15]. The first level is a client application designed to perform two functions: convenient setting of technological parameters of the polymer manufacturing process and access to computational results, including graphical and tabular presentation. The web interface is designed for usability, easy access and solving possible compatibility problems. After starting the front end of the information system, it is possible to select a task type and set all initial conditions for performing the process (Figure 2). After all possible parameters for solving the problem are initialized, the problem can be placed in the computation queue. For this purpose, a new entry is made in the database. It signals an unsolved task for computation, followed by depositing a set of initial conditions and defining input parameters for performing computations.

	128
Itanium-based isoprene polymerization in the reactor cascade	
typeAC_polymer	
Main parameters	~
AC type number*	
2	
Regulator number* 1	
Process maintenance mode	
○ periodic	
Modelling time*	
3600	
	~
reed stock composition	
Monomer concentration	
1.388	
IIBA concentration	
0	
Catalyst concentration	
0.0028	
AC share [%]	
2.2	

Figure 2. Web interface of the remote computing system frontend.

The second level is a system that allows storing all information in the database. It first stores the results of calculations for the corresponding problems and all necessary reference data, including various constants that determine the rate of chemical reactions. Since promising researches in this field do not exclude a possible simulation approach to modelling [16-17], it is more reasonable to physically split this layer and present it as a separate server. Of particular importance in the data storage system is a table that contains a list of all tasks that have been previously scheduled for execution or are currently scheduled. Each task has a status indicating its current position ("not started", "in progress", "calculation completed"), which allows you to examine the current state of the task queue.

The third layer (the base) is the calculation management system, which is responsible for performing the calculations required for a client. It is exactly the layer that controls all calculations and should be maximally prepared to perform resource-intensive tasks. This layer is represented by two levels of work management. The first layer is a control program that interacts with the database and periodically accesses its records to check if there are tasks to be performed. As soon as a new task shows up with the status "not started", it is executed, if resources are available, by one of the predefined executables located on the second level of this layer. The second layer contains pre-built bin files aimed at executing a specific and rather narrow computational task. The front-end, in turn, analyzes changes in the status of the assigned tasks in the background. When the status changes to "completed", it sends the results to the client. The described scheme of system operation is shown in Figure 3.



Figure 3. A conceptual scheme of the remote computing management system.

The layer responsible for computations works asynchronously with the system front-end. The reason for this is to continuously monitor the available computational resources required to perform the task. The drawback of this process is the need to control and mobilize resources to solve the task. These parameters are set and monitored by a software developer.

2-3- Solutions used in the Development

The front-end is written in Blazor C# [18], a UI framework for building interactive applications that run on the NET platform on both the server and client sides. The emerging task of visualizing the results is solved using the graphics library *Plotly.js*, which allows to create graphics directly in the client's browser and distribute the load of the data transmission channel. The application can run on mobile devices used as front-end computers.

The database management system that governs the operation of the system is the document-oriented DBMS MongoDB [19, 20]. Its choice is justified for several reasons. First, this DBMS is well scalable and supports a function such as" Sharding" [21] to begin with. Using this method, multiple tables of a single database can be distributed among multiple servers. Despite the physical distance between them, these tables are represented as a single record during processing. Sharding simplifies data processing when the database is limited in terms of storage space and processing power. Second, the DBMS supports the replication feature, which keeps database copies on two physically remote servers and sets duplication rules for the second database if changes are made to the first. In the future, this will simplify the operation of a hybrid cloud where some computations are performed locally and some are performed remotely with duplication of the changes in the database.

The bin file library is a repository of executables that any developer can participate in creating, as the system is not tied to any particular programming language. In particular, all developments to solve direct prediction problems are currently written in Python. The launch of all authorizations in a remote space is managed using Docker container technology. This is an operating system level software virtualization whose core is responsible for this. Managing virtual isolation of resources is necessary so that concurrently running applications cannot affect each other in any way. The main challenge in designing such an architecture is to allocate computational resources wisely to perform several elementary computations based on the GPU. At the moment, a CPU core is used to solve a similar task. The main research methodology can be represented in the form of a flowchart (Figure 4).



Figure 4. The main research methodology as a flowchart.

3- Results and Discussion

The remote computing system was tested by a computational experiment to determine the molecular parameters of the isoprene polymerization product produced by a continuous method in the titanium-based catalytic system. The conditions of the computational experiment were set based on real operating production and have the following technological characteristics:

- The catalytic system consists of 4 components *TiCl*₄-TIBA-Pip-DFO.
- The catalytic system component ratio of $TiCl_4/Al(i-C_4H_9)_3/Pip/DFO = 1/1/0.2/0.15$ mol.
- The number and type of reactors in the continuous production cascade is2 ideal mixing reactors with a working volume of 16.6 m³.
- The mass flow of polymerization products is 19 t/h at a monomer load of 5.4 t/h.
- The titanium catalyst rate was 1 mol $TiCl_4/980$ mol of isoprene.
- Diisobutylaluminium hydride (regulator) is not supplied.
- Molar concentrations of the reagents used: isoprene-1.388 mol/l; TIBA-0.0014 mol/l; active centers 0.0028 mol/l.
- The average residence time in one polymerizer is 30 minutes (60 minutes for the entire cascade).

The computing management system was hosted on a server with two processor modules of 18 cores each, a base clock speed of 2200 MHz, 64 GB of RAM. The calculations did not use the video card. All the data was stored on a stationary personal computer running a 4-core processor with a base clock speed of 2600 MHz. There was a 250 GB SSD and two 3.5" HDDs with a capacity of 1TB operating in the RAID mode. The frontend characteristics are not significant for the system operation. The network is based on the wired data transfer technology with a rate of 100 Mbps. To provide a full load of the computing server, a task statement was simulated from 15 frontends at once. Compiled Python code was used as an executable file for conducting calculations.

The calculation results in the form of dependences of the average calculated and average mass molecular weight on time are shown in Figures 5 to 6. For ease of viewing, the dependencies are given both on time and in the context of each polymerizer. The dots on the graphs indicate the results of laboratory experiments aimed to assess the data consistency. Previous research [20] observed other dependencies for the same experimental conditions based on a stationary calculation system scheme.



Figure 5. The dependence of the calculated average molecular weight on time for polyisoprene on the catalytic system *TiCl*₄-TIBA-Pip-DFO (line denotes the results of calculations, dots show the results of a laboratory experiment).



Figure 6. The dependence of the calculated weight-average molecular weight on time for polyisoprene on the catalytic system *TiCl*₄-TIBA-Pip-DFO (line denotes the results of calculations, dots show the results of a laboratory experiment).

The calculation time lasted from 3.11 to 3.87 seconds for each frontend. A similar task in terms of using a standard calculation system (by means of a local PC) required 28.12 seconds for the computer operation and provided the same results. Task queueing was checked by a script written for automatic task settings to be performed at different time intervals. The many-hour operation mode showed the successful performance of all the tasks within the allotted time. A similar computational experiment was carried out for the mono-center catalyst with a more extended kinetic scheme:

- The catalytic system *NdCl*₃- nIPA-TIBA-Pip.
- The ratio of the components of the catalytic system $NdCl_3$ /TIBA/Pip = 1/12/2 mol.
- The number and type of reactors in the continuous production cascade is 3 ideal mixing reactors with a working volume of 16.6 m³.
- The mass flow of polymerization products is 20 t/h at a monomer load of 4.2 t/h.
- The titanium catalyst rate was 1 mol NdCl₃ /10 000 mol of isoprene.
- The supply of diisobutylaluminium hydride (regulator) is 0.04 kg per 1 ton of monomer.
- Molar concentrations of the reagents used: isoprene-1.39 mol/l; diisobutylaluminium hydride 0.000177 mol/l; active centers 0.00014 mol/l.
- The average residence time in one polymerizer is 28 minutes (75 minutes for the entire cascade).

Simulated calculations from 30 client locations took 52.2 seconds of computer operations under the standard computation system (by means of a local PC). While calculations in a remote computing system required only 4.93 seconds. The results of the calculations are shown in Figures 7 to 8.



Figure 7. The dependence of the calculated average molecular weight on time for polyisoprene on the catalytic system *NdCl*₃-nIPA-TIBA-Pip (line denotes the results of calculations, dots show the results of a laboratory experiment).



Figure 8. The dependence of the calculated average molecular weight on time for polyisoprene on the catalytic system *NdCl*₃-nIPA-TIBA-Pip (line denotes the results of calculations, dots show the results of a laboratory experiment).

Similar calculations were carried out by means of a local PC [22, 23], their findings completely correspond to the calculated data of the present study. More large-scale tasks with the higher number of CPU cores can provide a broader outlook on the advantages of the suggested approach. In particular, optimal parameters in polyisoprene production based on a neodymium-containing catalytic system were studied to get a product with a given molecular weight using the genetic approach [24]. The remote solution of this problem in the same search conditions by selecting better production parameters and solving problems with different initial conditions provided a similar result in a shorter time. However, these calculations require the processor core parallelizing. Indeed, not every task can be divided into elementary subtasks having no intermediate data for a certain period.

4- Conclusion

The proposed approach and the developed remote computing system enable more efficient use of computer resources and significantly reduce the computation time in several of typical research tasks, which is confirmed by the results of the conducted computational experiments. According to the network architecture of the proposed system, the computational and data storage layers are physically separated. A unified database is developed for further laboratory and computational experiments to solve promising problems in using neural network technologies in chemical kinetics problems [25, 26]. Moreover, the proposed unified approach to problem formulation, condition description, and model construction eliminates the need for a routine mathematical description of the process, since all possible processes are already embedded in the system. This approach makes it possible to use the developed network tools both for experts in the field of modelling and for college students to conduct numerical research. The system supports the introduction of additional computational modules for new calculations and is not limited to solving direct problems in chemical kinetics. In addition, in multi-user mode for performing calculations, the system allows the use of all the capabilities of a high-performance cluster from multiple workstations in the mode of full resource utilization 24 hours a day.

5- Declarations

5-1-Author Contributions

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

5-2-Data Availability Statement

The data presented in this study are available in article.

5-3-Funding

The study was carried out within the framework of the state assignment of the Ministry of Science and Higher Education of the Russian Federation (scientific topic code FZWU-2020-0027).

5-4- Conflicts of Interest

The authors declare that there is no conflict of interests 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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