Research aspects of modeling and automated process control photopolymerization

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Abstract. This paper provides an overview of the state of existing systems of predictable control of the polymerization process. It includes a literature and patent survey of the presented mathematical models of the processes that occur during chemical polymerization reactions and analyzes techniques of controlling the processes of designing, manufacturing, modeling and construction of automated control systems. A critical analysis of existing modeling and control systems is given. The most promising software complexes ready for use in the process of designing of materials and products from photopolymers with predetermined structural properties have been identified. The analysis of a standard technological process as an object of control, by the example of the presented algorithm of the functioning of a particular production unit, showed the possibility of improving the existing automated systems of its control. By this example the authors prove the possibility of constructing automated process control systems, as well as those of photopolymerization, which will stabilize physical and chemical processes when manufacturing products from photopolymers. At the end of the research it was made possible to determine the purpose and objectives of further research of the authors aimed at creating the following complex: a software for the development of materials with specified structural properties; development of mathematical tools for calculation and modeling of photopolymerization processes; construction of automated control systems for technological processes of manufacturing products from photopolymer structural materials.

1. Introduction
The fact that photopolymers are insufficiently used in mechanical engineering unreasonably limits its capabilities and, as a consequence, the competitiveness of products, especially in the transport industry. Earlier studies conducted by the authors [1] showed that the main factor restraining the introduction of products made from photopolymers as structural materials is their low hardness. Therefore, the purpose of these studies was to investigate the state of affairs in modern science and technology during the design of the creation and production of polymers with predetermined structural parameters. Achieving this goal requires the study and analysis of existing methods and techniques of the process of modeling polymeric materials.

2. Analysis of existing methods and techniques of obtaining polymeric materials
Having considered the existing possibilities of scientific and technological advancements in modeling and obtaining new polymeric materials, it was concluded that they are based on a number of mathematical models and software packages (SP) (fig. 1).
After analyzing the existing software packages for modeling polymeric materials, it was determined that the most common software are GROMACS and LAMMPS (fig. 1 a, b). Nevertheless, the discussion of their popularity in the Internet community showed that finite-simulated courses for them are extremely difficult to perceive and time-consuming.

The presented software packages ALEO and ALEO-DIAGNOST (fig. 1 c) make it possible to obtain and calculate the necessary parameters of the equipment during heating or when diagnosing the quality of the polymers produced, but it does not provide for the possibility of working with the polymerization process of thermosetting materials.

The considered software package, namely, that of the OCTA program, discovered that they are a set of motors for modeling the polymerization process allowing one to work at different scales. Also there is an option of rough (enlarged, accelerated) grain modeling in this software. Consultations with experts showed that although the software considered is not a sufficiently flexible model, and it is extremely difficult to use the software to simulate the photopolymerization process, it can be used as an approximate simulation of the process.

The analysis of software packages showed that in an explicit, visualized form, the process of creating photopolymers with specified structural parameters is not represented in them. In this regard, additional research was carried out in the field of available mathematical models of photopolymerization processes.

Having conducted a literature and patent survey of existing mathematical models, it was determined that their number is extremely limited and they are aimed mainly at calculating temperature regimes in the field of reactors. The modeling of the process of electrothermal treatment of thermoplastics is elaborated mathematically in sufficient detail \([2...7]\) in order to maintain stabilized heating with their parameters changing during processing, but these mathematical models are limited only to the method of heating using internal heat sources.

The most suitable model \([8]\) describes the polymerization process of the substance by the example of 9 - vinylcarbazole with DEAX. It shows the possibility of interpolation at finding unknown intermediate values of the material concentration during the polymerization process.

The analysis of the model shows that it proceeds in two stages:

1. **I stadia:**
   \[
   \text{BK} + \text{DEAX} \xrightarrow{k_1, k_2} \text{[BK...DEAX]},
   \]
   where VC is 9-vinylcarbazole and [VC ... DEAX] is the complex system.

2. **II stadia:**
   \[
   \text{[BK ... DEAX]} \xrightarrow{k_2} \text{[P+AlEt_2Cl_2]} + \text{BK},
   \]
   \[
   \text{[P+AlEt_2Cl_2]} + \text{BK} \xrightarrow{k_5} \text{polymer},
   \]
   where [P+AlEt2Cl2] is the complex compound.

The authors describe chemical reactions by a system of differential equations of the following kind:
\[
\begin{align*}
\frac{dc_1}{dt} &= -k_1c_1c_2 - k_3c_3c_4 \\
\frac{dc_2}{dt} &= -k_1c_1c_2 \\
\frac{dc_3}{dt} &= -k_2c_2c_1 - k_3c_3 + k_4c_4 \\
\frac{dc_4}{dt} &= -k_4c_4c_1 + k_3c_3 - k_4c_4 \\
\frac{dc_5}{dt} &= -k_5c_5c_4
\end{align*}
\]

with initial conditions:

\[c_1(0) = c_1^0, c_2(0) = c_2^0, c_3(0) = c_3^0, c_4(0) = c_4^0, c_5(0) = c_5^0,\]

where \(c_1(t), c_2(t), c_3(t), c_4(t), c_5(t)\) – is the concentration of chemicals: VC, DEAX \([\text{VC ..., DEAX}, [\text{P+AlEt}_2\text{Cl}_2]\]; k_1, k_2, k_3, k_4, k_5 – are the kinetic parameters of polymerization of VC with DEAX in chloroform solution at stage I. The presented system of differential equations describes homogeneous thermodynamic polymerization reactions in a closed system \([9...12]\).

The mathematical model presented above makes it possible to calculate the concentration of input materials in the polymerization process, but the authors by no means indicate the possibility of using it in the process of direct production. Thus, it can be concluded that the presented mathematical model is of interest only as an academic development.

It should also be noted that, as a rule, the algorithms of the technological process do not provide for the possibility of including the modeling process in its control system.

Thus, the next stage of research was aimed to determine whether it is possible to control technological systems of polymer production, as well as to consider existing or proposed automated control systems (ACS) for polymerization processes used in industry.

3. Analysis of technological processes of polymer production as an object of automated control

The conducted researches and analysis of ACS systems have shown that automation of polymerization processes is at a fairly high level. Almost all electrophysical parameters of the production process are monitored in real time. Nevertheless, in practice, in the production and operation of products made of polymeric materials, their instability of mechanical, physical and technical indicators is detected. For example, defects in the production of PVC products \([13...18]\) reach 18% due to different properties of input raw materials (in terms of declared passport data) and instability of the conditions of the technological process.

After conducting a literature survey of existing algorithms of controlling the polymerization process of the substance, it was also found that they are not fully highlighted in print. Their number is very limited, and the presented ones are mainly built according to a standard scheme, an example of which is the algorithm \([13...18]\) discussed below.

The algorithm describes the key technological parameters of the process (fig. 2). It is based on the scanning of sensors of flowrate and the composition of "polymerizer-first stage degasser" systems. Its advantage is that the implementation takes place in a distributed control system in real time (by the example of the BK PAO Nizhnekamskneftekhim plant):
Figure 2. Algorithm of controlling the process of polymerization of butyl rubber
where $\Delta t$ is the period of scanning of sensors of flowrate and composition; $N$ is the number of sensor scanning per day of the polymerization cycle; $M_{\text{polym}}$ is the amount of polymer obtained from one polymerization system per unit time; $i$ - the numbers of polymerization reactors that are in the running cycle on the design day; $C_{\text{isob.}}$ is the concentration of isobutylene in the furnace charge, % wt; $L_{\text{ch}}$ is the furnace charge consumption in polymerizer, kg/h; $L_{\text{kat.}}$ is the total consumption of catalyst solution (large + small circuits), kg/h; $CAICl_3$ is the concentration of aluminum chloride; $C_{\text{st}}$ - is the concentration of calcium stearate in suspension.

Analysis of the presented algorithm shows that it is possible to use it as a standard one, but only with a number of assumptions in relation to the conditions of specific enterprises. Nevertheless, there are signs of universality in it. This algorithm makes it possible to determine the concentration of the substance at the intermediate stages of polymerization shown by the example of the concentration of calcium stearate (1).

$$C_{\text{st, Ca j}} = \frac{L_{\text{sysp j}} C_{\text{st, Ca j}}}{0.03L_{\text{XM j}} + M_{\text{polym j}} + L_{\text{sysp j}} C_{\text{st, Ca j}}}$$  
(1)

It also fully confirms the possibility of further automation of the processes of obtaining polymers. At the same time, when building new process control systems, it is necessary to adhere to the principle and conditions of the full integration of automated control systems into existing control systems [15].

4. Conclusion

Having conducted a literature and patent survey of existing mathematical models and polymerization algorithms, we can conclude that:

- existing software complexes for the development of materials with specified structural properties do not make it possible to organize the process of manufacturing products from photopolymers;
- the mathematical tools for calculating and modeling polymerization processes is shown in the academic literature only by individual developments, photopolymerization models are not presented at all. Mathematical models are not systematized and most often represent only academic interest;
- despite the high degree of automation of technological processes for the production of polymeric materials, problems associated with the quality of products are detected, especially in the manufacturing of products from structural polymers;
- analysis of technological processes of production of polymeric materials as control facilities shows their openness to the further construction of automated control systems.

Thus, the conducted studies have shown that the actual tasks of subsequent research are the works on the development of a mathematical model and automation of the process of obtaining products from a photopolymer with specified structural properties, which is the purpose of further research of the authors. Results of these researches will be highlighted by them after the works are carried out.

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