Optimization of control of chemical and technological processes of mixing and structuring multi-component elastomeric composites based on mathematical modeling methods

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Abstract. The work is devoted to the actual problem of optimizing the control of complex chemical-technological processes of structuring multicomponent elastomeric composites. Optimization of production processes improves the quality of the products obtained, contributes to their intensification, as well as reducing the formation of defect. The article discusses the optimization of the process of structuring multicomponent elastomeric composites based on physicochemical representations and kinetic mathematical models. The basic relationships between model parameters and quantitative characteristics of the process of structuring elastomeric composites are given. It is shown that, along with the main characteristics of the structuring process, it is advisable to use new quantitative estimates - the amplitude and mode of the velocity curve. An optimization criterion is formulated - increasing the economic efficiency of production of products from elastomeric materials by increasing the percentage of obtaining high-quality products from raw materials while minimizing defect.

1. Introduction

Modern processes for producing products from multicomponent elastomeric composites are characterized by complexity, multi-stage and scale production. Production processes include: the preparation of rubber and ingredients; their weight; in fact, the process of mixing rubber with ingredients, leading to the formation of an intermediate product - crude rubber mixture, semi-finished product; structuring process; as well as control and management of the processes of mixing and structuring of elastomeric composites at the stage of the rubber mixture and the finished product [1, 2].

Strict adherence to the parameters of production processes is necessary to obtain high-quality finished products with the required set of properties. The most critical technological stages of product manufacturing are the processes of mixing and structuring of elastomeric composites [1].

The organization of management and control of technological processes for the production of elastomeric composites, such as mixing and vulcanization (structuring), is currently based on the analysis of rheograms of the states of multicomponent elastomeric composites. State rheograms are obtained on rotor and rotor-free type vibroreometers. Modern rheometers are complex instruments that accurately describe the behavior of an elastomeric composite at all stages of its processing. Moreover,
for the successful management of the production processes of mixing and structuring elastomeric composites, the qualitative interpretation of the results of rheometric studies is fundamental.

2. Main part

Processing the data of vibration testing is a separate, rather complicated task [2, 3]. A large array of experimental data makes it possible to approximate the dependence of the torque $M_{kr}$ (the main characteristic of the process) from time to time by mathematical models and establish the main quantitative relations between the model coefficients and the vulcanization characteristics: the time of structuring start $t_s$, half-conversion time $t_{50}$, the optimum structuring time $t_{90}$ and the degree of completion of the process $\beta$. Torque dependence $M_{kr}$ from time can be expressed as follows:

$$M(t) = a + b \left( 1 - \left( 1 + \exp \left( \frac{t + d \cdot \ln \left( \frac{2^{1/e} - 1}{c} \right)}{d} \right)^{-e} \right) \right).$$

This model is numbered 8092 according to the catalog of Table curve 2d (SYSTAT Software) [3]. Parameter $a$ corresponds to the minimum torque $M_L$, parameter $b$ to the increment of torque $M_{H} - M_{L}$, and parameter $c$ to the vulcanization characteristic $t_{50}$. The parameters $d$ and $e$ are related to each other and to the vulcanization characteristics by the following relationship:

$$t_{C(90)} - t_{C(10)} = d \cdot \ln \left( \frac{10^{1/e} - 1}{10^{1/e} - 9^{1/e}} \right) + \frac{d}{e} \cdot \ln 9.$$  

Passing to the degree of vulcanization $\beta = (M - M_{min}) / (M_{max} - M_{min})$, we obtain the ratio for the generalized rheogram of the state ($\beta \in [0; 1]$):

$$\beta = 1 - \left( 1 + \exp \left( \frac{t + d \cdot \ln \left( \frac{2^{1/e} - 1}{c} \right)}{d} \right)^{-e} \right).$$

where $\beta$ is the normalized dimensionless quantity that characterizes the degree of completion of the structuring process.

![Figure 1. Approximation of the rheogram of the state of the elastomeric composite by model 8092.](image-url)
Table Curve 2d allows you to calculate model parameters. The five-parameter model 8092 we have chosen is non-linear with respect to the parameters. The Table Curve 2d program allows, along with the usual structuring curve, to obtain the process speed curve - the derivatogram of the process. Figure 2 shows the result of constructing such a curve.

Such differential process velocity curves (derivatives) in the Table Curve 2d program are described by model 8062:

$$ V = \frac{A}{D} \left( 1 + \exp \left( \frac{t + C \cdot \ln(D) - B}{C} \right) \right)^{-\left(\frac{D-1}{D}\right)} (D + 1)^{\left(\frac{D-1}{D}\right)} \exp \left( \frac{t + C \cdot \ln(D) - B}{C} \right). $$

In this relation, $A$ is the amplitude of the velocity curve (maximum velocity value), $B$ is the mode (abscissa of the maximum velocity) [3-5].

The parameters of the differential model are expressed as follows in terms of the parameters of the integral model:

$$ A = \frac{b}{d} \left( \frac{e}{e+1} \right)^{e+1}; \quad B = c - d \cdot \ln \left( e \cdot \left( 2^{1/e} - 1 \right) \right); \quad C = d; \quad D = 1/e. $$

Differential velocity curves of the structuring process are widely used in the analysis and control of the process, because they are more sensitive to changes in the levels of prescription and technological factors [5].

Management in the processes of mixing and structuring of elastomeric composites today is management by indirect indicators - individual characteristics for each mixture, which are found by analyzing state rheograms. The data obtained during vibro-rheometric tests are the basic information necessary for the operator-technologist to make operational decisions on monitoring and control of the process.

The constructed mathematical models reflect the state of a multicomponent elastomeric composite at the technological stages of mixing and structuring, preceding the receipt of the finished product.
and, therefore, can be used to predict the behavior of these processes, as well as directly for their optimization.

Optimization of production of products from elastomeric composites involves, first of all, the competent organization of management and control of technological processes for the production of elastomeric composites, such as mixing and vulcanization (structuring). Optimization in this case is aimed at maximizing the profit obtained by increasing the percentage of output of high-quality products from raw materials while minimizing costs by reducing rejects due to more flexible and operational control and management of mixing and structuring processes based on the analysis of state rheograms and constructed kinetic models of processes.

To optimize the control of mixing and structuring of elastomeric composites, it is proposed, in addition to the traditional basic indicators of the structuring process ($t_s$, $t_{50}$, $t_{90}$), to additionally consider such quantitative characteristics of the process as amplitude $A$, mode ($M_0 = B$), calculated on the basis of the coefficients of mathematical models [6]. At the same time, the total number of control points necessary for more flexible and efficient control and management of the processes of mixing and structuring of multicomponent elastomeric composites increases. Such a set of quantitative characteristics (taking into account new parameters) allows you to uniquely identify the rubber mixture (its composition and processing parameters into the product) based on the calculated coefficients. Given the large number of formulations used in the rubber industry (more than one and a half thousand), these quantitative characteristics are individual and unique for each mixture, in contrast to state rheograms. In view of the foregoing, in order to increase the efficiency of the work of a chemical technologist’s operator, it is necessary to create a database for managing complex chemical and technological processes of mixing and structuring multicomponent elastomeric composites, in which new quantitative characteristics will be stored. The accumulation of such information about these processes will make it possible to more accurately establish confidence intervals for the parameters of processing elastomeric composites into finished products, which will help to improve its quality.

3. Conclusion
The analysis of the state rheogram and the construction of a mathematical model allows us to predict the course of the structuring process and makes it possible to identify, analyze and form various technological situations in the production of products from elastomeric composites, which allows individually, using modern digital technologies, to solve the problem of optimizing the mixing and structuring of multicomponent elastomeric composites, taking into account the large number of formulations used in the rubber industry.

References
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