

## MATHEMATICAL SIMULATION OF SOLID PHASE EXTRUSION OF COMPOSITE MATERIALS

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**Key words and phrases:** boundary and initial conditions; isometric and non-isometric processes; mathematical model; mathematical simulation; rheological characteristics; solid-phase extrusion; SHS-extrusion; technological process; thermal model.

**Abstract:** The work expounds the basic aspects of mathematical simulation of the process of solid phase extrusion of composites. It reviews the approaches, ideas and methods of the mathematical simulation that are equally useful for SHS and other processes of chemical technology. One gives the example of successful application of mathematical simulation for specific practical recommendations and prognosis of problem situations in the technological practice of SHS-extrusion.

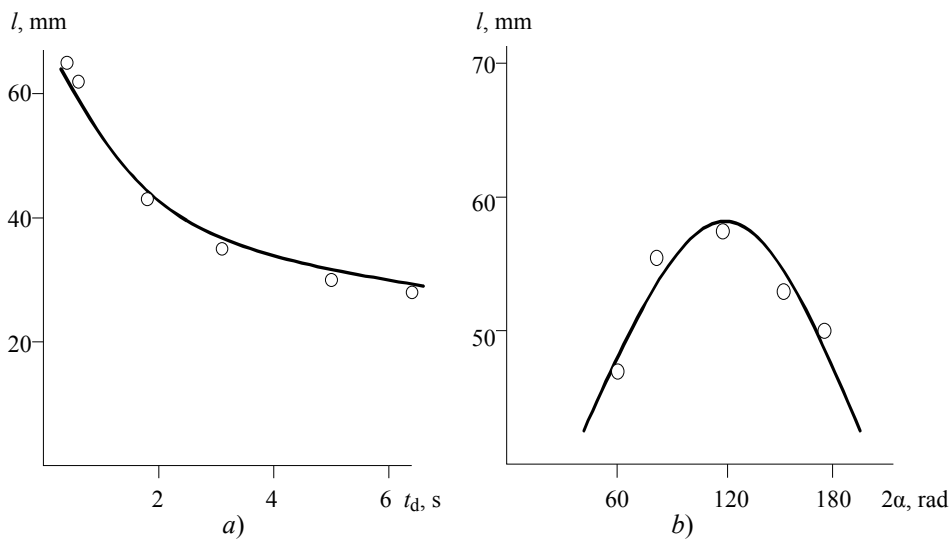
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### Introduction

During the processes of solid phase extrusion (including SHS-extrusion) a high-melting material is synthesized fast (about one minute). The processes are accompanied by such interior heat development (instead of external one) that the material is transferred to the plastic state under the external pressure. The general peculiarity of the methods is the combination of burning and high-temperature deformation [1–2]. The first tests on the experimental process flow diagrams have displayed the necessity of matching the technological parameters with some optimal ranges. The method of mathematical simulation, in this case, proved to be highly effective. It has allowed to calculate optimal parameters of a process at production of specific articles from various materials, to avoid the problem situations and to predict the results of experiments.

#### 1. Analysis of basic stages of a technological processes

Any technological process represents a set of technological operations corresponding to the basic stages of the process. The stages can be marked on the time charts of the process (Fig. 1, *a*). For example SHS-extrusion of powder-materials includes the following three stages : combustion and delay, compaction, and extrusion.



**Fig. 1. Dependence of the length of the squeezed out part of a sample  $l$ :**  
*a* – on the time of delay  $t_d$ ; *b* – on the angle of conical fuzz of a die  $2\alpha$ ;  
the smooth line is drawn theoretically, the points – experimentally

The peculiarity of the suggested method is the allocation of self-contained sequentially proceeding physical stages. Each of them is analyzed in detail taking into account its specific objectives and peculiarities. Theoretical analysis of any consequent stage takes into account the results of the previous stage analysis in the form of initial conditions. The advantages of such an approach were accepted not long ago and widely used in the polymer processing theory.

At the first stage the synthesis of high-melting compound takes place. The stage of compaction includes the compression of exothermic reaction products due to the reduction in the volume of entrapped air in the material and macrospores closure. Presence of the stage is due to the compressibility property of the powder material. At the stage of extrusion two important problems are being solved. They are molding and refrigeration. The diversity of the article configurations is achieved with the shape of a die through which the material is forced. Thus, at the third stage the flow of the material occurs. Its regularities mostly depend on the rheological properties of the material. At the solidification of the material at the expense of refrigeration it is important to avoid heat stresses in a sample and in walls of a mould.

The peculiarities mentioned above determine the specific character of self-contained theoretical analysis of thermal conditions at each of the stages. Such analysis must be taken into account when formulating the mathematical models.

## 2. Formulation of mathematical models of solid-phase extrusion

An important aspect of mathematical simulation of a specific technological processes is the use of specific data on the real conditions of the process that were formally derived in the theoretical researches on SHS-processes. One should emphasize the prevalent application character of the researches in the field of mathematical simulation. The researches are characterized by their all-round use for solution of specific technological problems. At the same time one have discovered a necessity to supplement the obtained knowledge with that from the field of powder material mechanics in general and the rheology of the materials in the field of high temperatures in particular.

It can be mentioned that the key to success for any technology of receiving finish products is rheology, i.e. the science dealing with the deformation and fluidity of materials. With reference to the process of solid phase extrusion one puts on the foreground the problems of rheokinetics, concerned with study of rheological properties of a changing system.

As the main parameter of thermal models they chose the temperature, that is the function of three coordinates and the time  $T = T(r, z, \phi, t)$  ( $r$  – radial,  $z$  – axial,  $\phi$  – angular coordinates). The leading hand of the parameter is implied by a large temperature diapason about 2000...3000 K. For solution of a specific thermal problem it is necessary to determine the geometry of the body, boundary conditions and physical properties of the material.

The process being researched can be described by the system of differential equations for:

– a heat insulator (1):

$$\frac{\partial T_1}{\partial t} = a_1 \nabla^2 T_1 = a_1 \left( \frac{\partial^2 T_1}{\partial r^2} + \frac{1}{r} \frac{\partial T_1}{\partial r} + \frac{\partial^2 T_1}{\partial z^2} \right);$$

– a sample (2):

$$c \left( \frac{\partial(\rho T_2)}{\partial t} + f(\rho, z) \frac{\partial T_2}{\partial z} \right) = \lambda_2(\rho) \nabla^2 T_2;$$

– and a mould (3):

$$\frac{\partial T_3}{\partial t} = a_3 \nabla^2 T_3 = a_3 \left( \frac{\partial^2 T_3}{\partial r^2} + \frac{1}{r} \frac{\partial T_3}{\partial r} + \frac{\partial^2 T_3}{\partial z^2} \right).$$

Depending on the stage of the process the functions  $f(\rho, z)$ ,  $\lambda_2(\rho)$  have the following values:

$$f(\rho z) = \begin{cases} 0 & \text{(combustion, delay);} \\ \frac{\rho U_n z}{H_0} & \text{(compaction);} \\ \frac{Q}{\pi R^2(z)} & \text{(extrusion);} \end{cases}$$

$$\lambda_2(\rho) = \begin{cases} \lambda_0 & \text{(combustion, delay);} \\ \lambda_0 \left( \frac{\rho_0(1 - U_n t / H_0)}{\rho_0} \right)^k & \text{(compaction);} \\ \lambda_k & \text{(extrusion).} \end{cases}$$

The results of the heat problem solution are the temperature fields in the sample, the heat insulator, the mould, the part of material being molded and the predicted length of the final product. The extrusion stops when the part of the material, located in the profiling die and directly over its orifice, loses its 'vitality', i.e. the capability of plastic deformation, and cork up the outlet. The received length,  $y$ -coordinate of the lower boundary of the sample, is the sought of the product.

In the thermal models the role of rheological factor is considered through effective characteristics – the temperature of 'vitality'. Though the models do not allow to rate

the processes of high-temperature deformation and compression, which key parameters are macroscopic density, speed and stresses in the material.

During synthesis of a material, its compaction and refrigeration, its ability to macroscopic flow sharply varies. Such an ability is determined by rheological properties of a hot porous mass. The porous material, transferred to a high-temperature condition, is rheologically insufficiently studied. Its specificity is the presence of great amount (up to 50 %) of pores, modification of the porosity during compression, and formation of a continuous frame from the particles of high-melting component in the field of pre-melting temperatures. Such a frame resists to the deformation. Non-isothermal rheodinamical models [6–14] have been designed for qualitative and a quantitative analysis of non-isothermal flow of compressible materials in different zones of SHS-equipment. The models were obtained by means of complication of those designed before.

The primal problem of theoretical rheodinamical models review is the analysis of density, temperature and intense-deformed condition of a material during its extrusion, depending on the pressure and the initial distribution of temperature and density in a sample. An important point of such exposition is the selection of the rheological equations. Further on it is supposed, that compaction of a material happens by the mechanism of frictional flow of a mass in pores (according to the Ja.I. Fraenkel theory). Rheological properties of such medium, i.e. ability to deformation and flow, are determined by properties of a solid phase, presence and a degree of porosity. For all such models the invariance of rheological relations is common. Such relations help to express the rheological properties of porous materials in terms of rheological characteristics of incompressible phase and some functions of porosity and temperature, defined in the experimental way [1–2].

### 3. Calculation of input data

One of the most laborious stages of mathematical simulation is the calculation of input data. Nevertheless their collection and analysis is a crucial part of simulation. A safe and consistent model should not contain so-called «free» parameters which are frequently used for adjustment of a model to experiments. It allows to apply the model to various experimental situations and to carry out direct comparison of the theory and experiments.

The development of a process depends on various modes of operation, exterior conditions, natural properties of a material, geometry of molding equipment and its characteristics. Influence of these factors should be reflected through the parameters of a model. Unfortunately concrete data (physical and chemical properties of a material – technological object), real conditions of a process (boundary and initial) and specific data about the operation mode, equipment (technological and geometrical parameters) are impossible to calculate on the base of literary information. In this case conducting of special experiments for definition of missing data is required. Other technique is rather useful. It consists in the introduction of so-called effective characteristics which reflect the influence of the whole set of parameters. For example in the special literature on heat-mass transfer they widely apply the effective coefficients of heat emission for simplification of the boundary thermal conditions.

One can allocate four basic groups of parameters. They are technological parameters, physical properties of a sample, characteristics of molding equipment, parameters defining the surface of interaction between a sample and the environment (boundary conditions). On choosing the optimal conditions of a process it's necessary to derive the value of each parameter from the four groups.

#### 4. Comparison of a model with the experiment

Comparison of a model and experiments should involve the characteristics that have complex nature. Good consent of the theory and experiments forms the foundation for multi-variant numerical explorations of thermal and rheodinamical conditions. For example, at the stages of combustion-delay and compaction (for SHS-molding, SHS-extrusion) they compare the temperatures in different points of a sample, a heat insulator and molding equipment (Fig. 1, *a*). At a stage of extrusion (for SHS-extrusion) the comparison is conducted longwise the squeezed out part of a sample (Fig. 1, *b*).

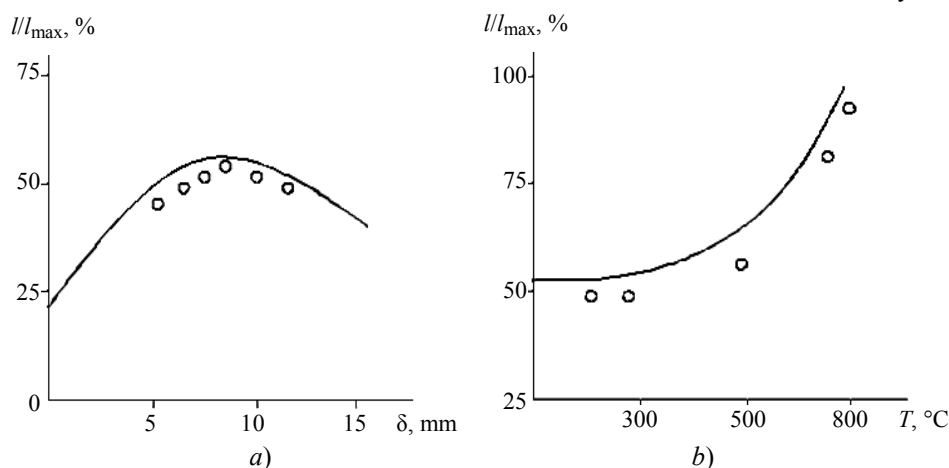
#### 5. About a possibility of prognosis

Use of a model for the prognosis and predictions is a challenge. One can say that the problem of the prognosis and optimization of a technological process is one of the main tasks of the mathematical simulation.

Works [3–14] expound the role of key parameters of a process, such as pressure on a plunger of a press, time of delay and exposure, geometrical sizes of a sample and a profiling lower die, deformation of a sample, etc. Dependences on some performances of the process are non-monotonic, that allows to mark the optimal ranges of the parameters. For example, Fig. 1 shows the angular dependence of length  $l$  of squeezed out part of a sample at extrusion ( $2\alpha$  is the angle of conical fuzz of a die). Non-monotonic character of this dependence has allowed to find out the optimal ranges of angles of the die ( $120^\circ \dots 150^\circ$ ) for deriving lengthy articles. For other parameters (such as the speed of a plunger of a press), which influence on characteristics of a process is monotone, limiting values were found out. Beginning with such a value the parameter does not influence on the characteristics of the process.

#### 6. Mathematical simulation for solution of repeatability problem

Results of mathematical simulation proved to be rather useful for solution of repeatability problem of a technological process. Such a problem is crucial for each method. Thus, for example, it was found out that the process repeatability of deriving of heating elements based on molybdenum disilicide by the method of SHS-extrusion is much lower than that of electrode elements based on carbide of titanium recieved by the



**Fig. 2. Dependence of relative length of the squeezed out part of a product  $l/l_{\text{max}}$ :**  
*a* – on the thickness of plug in the orifice of a die  $\delta$ ;  
*b* – heating temperature of a die and a gauge  $T$ ;  
the smooth line is drawn theoretically, the points – experimentally

same method. The analysis of temperature changes dynamics shows that the temperature ranges of material 'vitality' (i.e. the interval of processing) for heating materials makes 200...300 °C, and for carbide titanium hard-facing alloys is equal to 900 °C. Ranges of material 'vitality' can be defined as the difference between the temperature at the end of the compaction stage and temperature of 'vitality'.

Thus, molding of a material at deriving of heating elements is carried on close to the critical conditions, when a material loses ability to plastic deformation. Heat rejection in the orifice of a die proved to be a rather essential factor. Bringing the conditions of heat interchange on this boundary close to adiabatic sharply reduces the rate of refrigeration of a sample.

Influence of heating of a guiding gauge and a die on completeness of squeezing-out has been explored. Calculations have shown, that the heating of the gauge and walls of the die up to a temperature value belonging to some admissible ranges increases length of the final product. Thus, heating up to 500 °C increases the length in 1.7 times and heating up to 800 °C increases the length in 2.3 times (Fig. 2, *b*).

The conducted experiments have shown, that heating up to 250...300 °C increases the completeness of squeezing-out in 1.2 times, increases the density of the samples from 4.7...4.8 g/sm up to 5.1...5.3 g/sm, diminishes fissures and scales formation, and help to avoid blockage of the die [16].

## 7. Use of a model for quality improvement of received products

For the qualitative and quantitative analysis of non-isothermal flow of compressed materials in various zones of SHS-equipment non-isothermal rheodynamic models have been developed. The models were obtained by means of complication of the thermal models designed before.

The theoretical description is based on consideration of the equations of continuity, movement, rheological ratio and heat exchange.

The numerical decision of non-isothermal rheodynamic models results in defining of the unknown relative density, speed, temperature and stresses that are the functions of only one coordinate and the time. Criteria conditions have been found for the following modes of condensation: without condensation, incomplete condensation, condensation up to pore-free conditions, regular, wave and transitive modes of condensation. In the regular mode condensation occurs simultaneously throughout the volume of a material. Unlike the regular mode, in the wave mode disturbance from the plunger is distributed in layers and not instantly. In this case the speed of the wave of condensation is greater than the speed of the plunger. For transitive modes the wave of condensation degenerates, and the width of its front increases. This fact is promoted by smoothing of density on the ends of a sample.

## Conclusion

Mathematical simulation of a specific technological process should include the following stages:

- formulation of a mathematical scheme, relevant to the real conditions of the production (equipment, materials, process). An important part of this stage is the physical analysis of process and selection of key parameters of the model;
- calculation of specific data (physical and chemical properties of material-technological object), real conditions of the process (boundary and initial) and specific data on technological conditions and equipment (its technological and geometrical parameters);
- comparison of the model and experiments. It is important to establish the frames of the model application and its use for specific practical recommendations and prognosis of problem situations in technological practice;

– use of the results of mathematical simulation in engineering practice for deriving specific products.

The results, obtained in the field of mathematical simulation of various SHS-technologies, can be considered from the position of stages listed above.

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## Математическое моделирование твердофазной экструзии композиционных материалов

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**Ключевые слова и фразы:** граничные и начальные условия; изотермические и неизотермические процессы; математическая модель; математическое моделирование; реологические характеристики; СВС-технология; СВС-экструзия; твердофазная экструзия; тепловая модель; технологический процесс.

**Аннотация:** Изложены основные аспекты математического моделирования процесса твердофазной экструзии композиционных материалов. Рассмотрены общие подходы, идеи и приемы математического моделирования, одинаково полезные и для технологии СВС и для других процессов химической технологии. Приведены примеры успешного использования математического моделирования для конкретных практических рекомендаций и прогноза возникновения проблемных ситуаций в технологической практике СВС-экструзии.

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### **Matematische Modellierung der Hartphasenextrusion der Materialkomposites**

**Zusammenfassung:** In diesem Artikel sind die Grundaspekte der mathematischen Modellierung des Prozesses der Hartphasenextrusion der Materialkomposites dargestellt. Es sind die Hauptstandpunkte, Ideen und Verfahren der mathematischen Modellierung, die sowohl für SWS-Technologie als auch für die anderen Prozesse der chemischen Technologie ebenso nützlich sind, vorgebracht. Es sind die Beispiele der erfolgreichen Benutzung der mathematischen Modellierung für die konkreten praktischen Empfehlungen und für die Prognose der Entstehung der Problemsituationen in der technologischen Praxis der SWS-Extrusion angeführt.

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### **Modélage mathématique de l'extrusion des matériaux composites de la phase solide**

**Résumé:** Dans le présent article sont exposés les aspects essentiels du modélage mathématique du processus de l'extrusion des matériaux composites de la phase solide. Sont exposés les approches générales, les idées et les procédés du modélage

mathématique utiles pour la technologie et les processus chimiques. Sont cités les exemples de l'utilisation de modélage mathématique pour les cas concrets et pour les prévisions des situations problématiques dans la pratique technologique.

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