Journal of Engineering Physics and Thermophysics, Vol. 65, No. 1, 1993

MATHEMATICAL MODELING OF SHS EXTRUSION.
1. THERMAL MODELS

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UDC 621.7.011

A review of thermal SHS extrusion models is presented and their applicability for optimization of the process is discussed.

At present a new highly promising SHS extrusion method has been extensively used for production of elongated articles from refractory materials [1-3]. The method combines combustion and deformation. When mastering this method, process engineers encountered undesired effects of various origins such as very rapid material cooling, resulting in full or partial clogging of the die outlet, mechanical instability affecting the product quality, underpacking and supercompaction of the material, etc. [4, 5]. From the very beginning it has become evident that these serious situations can be eliminated with the aid of mathematical models for SHS extrusion process. Such studies were conducted simultaneously with an experimental investigation of the production regimes carried out by V. V. Podlesov, V. V. Vedeneev, and A. V. Radugin [1-2] and were very helpful for development of production processes for many articles such as electrodes for electric spark alloying and melting intensification, heating rods, rollers, etc.

In this article a procedure of mathematical modeling of SHS extrusion is presented. Ideas, approaches, and concepts are discussed, both general, borrowed from the theory of mathematical modeling, and specific for this process.

1. GENERAL PRINCIPLES OF MODELING EXTRUSIVE PROCESSES

Mathematical Scheme of SHS Extrusion. The model is formulated with the following assumptions. Let a chemically reacting substance fill the axisymmetric region G_2 (Fig. 1). The substance is confined by a thermally insulating shell that occupies the region G_1. The system studied is symmetric relative to the angular coordinate and it can be assumed that the variable process characteristics are functions of two coordinates (vertical z and radial r) and time t.

A flat combustion front moves down the specimen at a uniform velocity. The combustion front coordinate z is defined by $z_* = H_0 - U_c t$, where U_c is the combustion rate. Combustion takes place within the time interval $(0, t_c)$, where t_c is the combustion time. In the time interval (t_c, t_h) holding takes place until external pressure application. Then, the material is extruded by application of the plunger from the region G_2 to the region G_3 of the guiding pass, where the piece is molded.

Choice of the Model. SHS extrusion is complicated by many processes, namely, heat release, hydrodynamics, heat transfer, sintering, etc. Some rheological factors are important here since the object of deformation is a compressible refractory material. However, at the initial stage in the formulation of mathematical models, instead of creating a "universal theory" considering all factors affecting the process, an attempt was made to restrict oneself to a simpler mathematical scheme that includes only individual factors which control the process within a particular time interval. The starting point in the formulation of a model is the problem situation itself and goals and objectives of the study. For example, for studing rapid cooling of combustion products, which results in clogging of the die, thermal models are formulated [6] for which temperature was taken out of the parameters that determine the quality of a finished product (pressure, temperature, density). The leading role of the parameter is determined by a wider characteristic temperature range (from the combustion temperature to the ambient temperature). In this

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Institute for Structural Macrokinetics, Russian Academy of Sciences, Chernogolovka, Russia. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 65, No. 1, pp. 83-89, July, 1993. Original article submitted January 29, 1992.

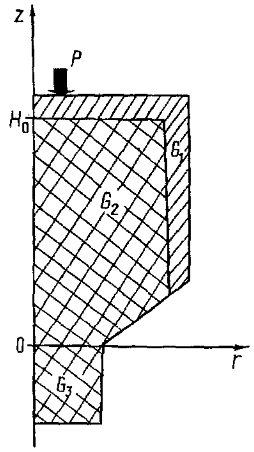

Fig. 1. The geometric region in which the problem is to be solved: G_1) shell; G_2, specimen in the mold; G_3) specimen in the pass (half of the region is shown in the figure).

connection, it seems to the point to recall the situation concerning the main ideas in the theory of combustion and explosion. The conclusion that it is heat conduction and not the chemical conversion mechanism that is of key importance in flame propagation seems quite evident and trivial at present.

To investigate compaction and extrusion of material and to answer the practical question about the time the material is compacted but not extruded or extruded without compaction, rheodynamic models were used with the main parameters of density, velocity, and stresses in the material [7].

Determination of the major stages of the process and their successive study are a main step. This approach substantially simplifies the mathematical models. On the one hand, the possibility of stage-by-stage consideration is implied by experimental realization of the process; on the other, this possibility should be shown theoretically by defining the criterial conditions for division into three stages. On the basis of time diagrams, three main stages of the process can be distinguished. They are combustion-holding, compression, and extrusion. In the first stage the material is synthetized from the initial components, while passing through the combustion wave. In the second stage the products of the exothermic reaction are compacted to the final density, usually close to the theoretical one. In the third stage the material is extruded out of the mold though a hole in the die into air or the guiding pass and the pieces are shaped.

The mathematical model should have the following properties:

1) it should suit a real process;

2) it should describe the qualitative effects observed in the experiment;

3) it should permit making preliminary conclusions and reducing considerably the amount of experimental work;

4) it should serve to justify the production methods employed.

With all these properties in view, we will discuss the most widely used SHS extrusion models.

2. THERMAL MODELS OF SHS EXTRUSION

Analysis of the Parameters in the Thermal Model. We will isolate four main groups of parameters which are vital for the SHS extrusion process. These are process parameters (pressure P on the press plunger, velocity of the plunger U_p, holding time t_h), thermal parameters of the specimen and shell, geometrical parameters of the press attachments (such as thickness of the mold walls, diameter of the opening in the die, and the cone angle of its bell), and parameters determining the thermal boundary conditions at the surface of the specimen, shell, and press attachments.

While being forced through the die, the material should have the capability of plastic deformation. The behavior of the material subjected to deformation depends on a set of rheological properties, primarily, on the viscosity and its dependence on the shear rate. However, within the model adopted the influence of rheological properties on the process is included indirectly, via the effective property of viability temperature (T_v). Simplification of the approach

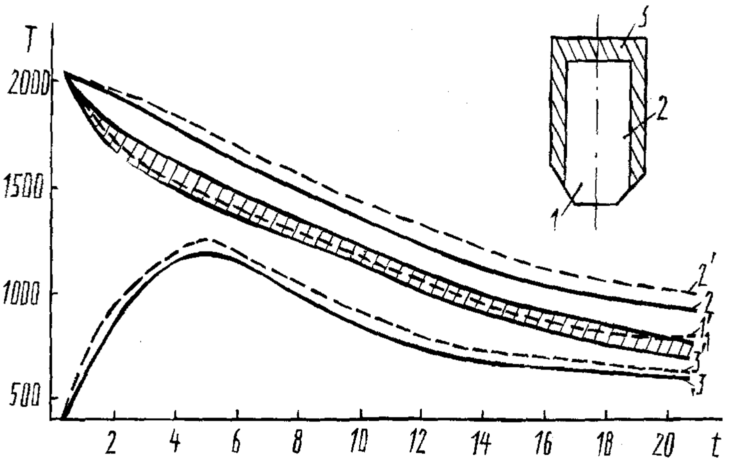

Fig. 2. Dependence of temperature T on time t at three different points, indicated in the scheme: 1) at the matrix wall; 2) in a specimen; 3) in the shell. Curves 1', 2', 3' are obtained experimentally; 1, 2, 3 theoretically. T, °C; t, sec.

consists in the fact that we not consider the dependence of the viability temperature on the set of rheological properties but assume that T_v is constant and to be determined experimentally. Thus, in the thermal models the role of rheological factors is simplified.

A quantitative description of the combustion process requires that the kinetic parameters of the chemical reaction be known. However, direct determination of the parameters is often very complicated. Therefore in the mathematical model the combustion rate U_c and the combustion temperature T_c are assumed to be parameters of the specimen combustion. These parameters can be determined experimentally under standard technological conditions of extrusion.

It should be noted that just as in any other theory employing effective parameters, these assumptions simplify considerably the mathematics of the problem. If we restrict ourselves to analysis of the thermal conditions of SHS extrusion, then as has been shown by experience in applying thermal models, such an approach appears reasonable. Thus, the model does not contain the so-called free parameters frequently used for correlation of the model and experiment. Because of this, the model can be used for various experimental situations, and direct correlation of the model and experiment can be made.

Statement of the Problem. For calculation of temperatures in the regions G_1, G_2 and G_3 a system of differential heat conduction equations is solved with the corresponding boundary and initial conditions presented in [8]. It will be noted here that two-dimensional unsteady-state problems with movable boundaries (the combustion front, the upper and lower boundaries of the specimen) are considered in complicated geometrical regions.

As a result of numerical computation, the temperature fields are found in all the regions in the material and the heat insulator. It should be noted that the temperature field formed at one stage is the initial condition for the subsequent stage. The computation results will allow the researcher to choose thermally optimal parameters and to predict the length of the product.

Thermal models formulated in this way have been used for the qualitative analysis of physically different regimes of extrusion of combustion products in the high-temperature region; with their help criterial conditions for their realization have been found.

Comparison of the Model with Experiment. A necessary component of mathematical modeling is comparison of the theory with practice, theoretical results with experimental data. It should be noted that in the development of thermal models comparison was made without fitting factors and the results agreed well qualitatively and quantitatively. Theoretical and experimental results were compared in terms of the time-temperature curve (Fig. 2) and the dependence of the article length on the delay time [8], the press plunger velocity, and the degree of deformation.

In Fig. 2, predictions are compared with experimental time curves of temperature at various points within the volume of the specimen and the heat insulator (the solid line is theory, the dashed lines are experiment). The good

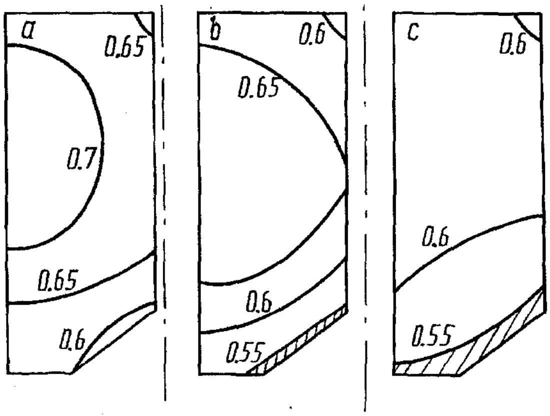

Fig. 3. Temperature fields in a sample formed 6 sec, 14 sec, and 18 sec after burning a pellet, corresponding to the various extrusion regimes: a) normal extrusion; b) partial clogging; c) complete clogging.

agreement of the curves confirms the chosen model. A comparison of theoretical and experimental results in terms of the dependences of the article length also showed good agreement [8]. After the comparison the model was used for explanation of various experimental situations, forecasts, and determination of thermally optimal process parameters.

Investigation. A computation experiment was very helpful for investigation of some important technological parameters [6, 8] such as the degree of deformation, pressure, and velocity of the press plunger, the cone angle of the die bell, and the delay time in order to determine their optimal range. It is a common situation that specific requirements on the product quality cannot be met by varying a particular parameter. Thus, the problem of choosing optimal parameters becomes ambiguous and has to be solved for each particular case from practical considerations.

In this respect, the analysis of the holding time (the time from the start of the SHS process to the time of the applying the pressure necessary for specimen degassing and forming the material structure) is very representative. On the one hand, an increase of the holding time, starting from 6 sec, ensures the condition of an optimum temperature range, thus facilitating the uniform distribution of the components within the product; on the other hand, it increases the completeness of extrusion. With this in view, it is recommended that a holding time of 2 to 6 sec be used.

Studies of the influence of the plunger velocity have revealed that this parameter simultaneously affects both the specimen cooling time, thus lowering the product quality, and the completeness of extrusion. Noticeable changes of the completeness of extrusion are found not over the whole velocity range, but only up to a certain value, which is equal to 20 mm/sec for extrusion into air. This value was taken as optimum.

Explanation of the Problem Situations. The mathematical models developed for SHS extrusion were very helpful in explaining some important problem situations that may be encountered in practice, when producing particular articles. For example, in experiments situations were observed in which the material was not extruded at all, or a specimen was extruded with a truncated top.

Analysis of the temperature fields in the chamber before extrusion enabled explanation of these effects from the thermal point of view. In Fig. 3 thermal fields are given for various times. The figure shows that it is possible that the die opening can be gradually clogged by cold material that lost viability (dashed areas in the figure). It follows from Fig. 3a that the mass at the outlet from the die has a temperature exceeding the viability temperature. As time passes (Fig. 3b), temperature of some of the material which is adjacent to the mold wall is reduced below the viability temperature T_v and the effective diameter of the opening decreases (partial clogging). As the holding time increases further, the die opening appears completely clogged by cold material (Fig. 3c).

There are examples where the model was very helpful for obtaining reproducibility of the extrusion process when producing heating elements from slowly burning compounds [8-10]. Analysis of numerical results enabled theoreticians to recommend that experimenters heat the die and pass, after which articles of larger length and better quality were produced, as was predicted by the theory.

Control and Design. The set of programs developed will be used for computer optimization of the SHS extrusion process. The procedure of using the programs consists of three stages: input of initial data; computation of temperature fields in the specimen, heat insulator, and mold for each of the process stages; display or printing of the information as graphs and tables. Before input of the initial data, it is necessary to determine the model parameters. Some of them are to be found by computation, others should be determined experimentally; technological and geometrical parameters should be specified. The program for computation of temperature fields for each of the stages is independent. Therefore it is possible to optimize the temperature fields for each stage separately, then to transfer to the next one by changing the initial data (different model parameters). After the necessary optimization, the temperature field for each preceding stage is taken as the initial condition for the subsequent stage. Computer investigation of SHS extrusion processes substantially reduces the volume of experimental work.

Design of Press Attachments. Mathematical modeling is very effective in designing press attachments and equipment. A set of programs for determination of the temperature fields in a specimen and the die as well as programs for computation of stresses in the mold were used for the development of a nonisothermal procedure for designing of press attachments, including specification of processes occurring inside the mold, namely, their essential instability, temperature nonuniformity and different levels of thermal gradients across the mold wall.

The following approach is ordinarily used in calculations of stresses in the mold walls [11-13]: a temperature drop that is assumed to be uniformly distributed across the wall is prescribed and the thickness δ is to be found at which the strength condition is fulfilled: the equivalent stress does not exceed the one allowable for a particular material. Thus, σ_{eq} is a function of pressure P, wall thickness δ, and temperature difference T: $\sigma_{eq} = f(P, \delta, \Delta T)$. If we take a real temperature profile, it usually appears that for SHS processes the temperature drop is localized in a narrow boundary layer, and it is not the whole wall that is subjected to thermal stress but a narrow part δ_1 of it. Therefore, for characterization of the thermal load of the whole mold wall it is useful to substitute the effective temperature $T_{ef} = \frac{1}{\delta}\int_0^{\delta} T dr$, determined as the integral mean temperature across the wall, in the expression $\Delta T = T_s - T_0$ in place of the temperature at the inner wall of the mold. Then the temperature drop across the wall will be $\Delta T = T_{ef} - T_0$. This substitution is physically reasonable since the part of the wall subjected to a high heat flux is much smaller than the part of it in which a considerable temperature gradient occurs: $\delta_1 << \delta_2$.

Furthermore, from the dependence of temperatures at the inner and outer wall surfaces on the wall thickness, we find the wall thickness at which the temperature does not exceed that allowable for a particular material of the mold, i.e., at which there are no structural changes in the material. For that particular thickness δ_T the temperature distribution inside the wall of the mold is calculated; then calculation of the equivalent admissible stress follows. Thus, while earlier δ_T was independent of the process conditions, now it depends on the particular process and not just on the temperature drop ΔT. Therefore, it is necessary to solve the thermal problem in the specimen in connection with that in the mold wall and hence to find δ_T.

Comparison of the results obtained with the isothermal and nonisothermal methods shows that the new procedure validates the use of molds with a smaller thickness of the walls with the same safety margin. It saves structural material and reduces the mass of elements with the safety rules being observed and the most unfavorable operating conditions being met. For example, a decrease of the mold wall thickness by only 5 mm permits a 15-20% reduction of its mass, which is equivalent to 200 kg for blanks with a diameter of 0.5 m and a height of 1 m. Reduction of material consumption for fabrication of press attachments is currently an urgent problem for SHS production methods.

Conclusion. The history of developing SHS extrusion is marked by a favorable peculiarity: relevant theoretical and experimental studies were conducted simultaneously and in interrelation. Each of the investigation methods had its methodology and encountered different difficulties. Within this review the authors did not discuss experimental and technological results, excluding the cases of direct comparison of experimental data with theoretical findings. The results given here are based on numerical computations following the thermal models developed. Today it can be concluded that such mathematical modeling has simplified labor-consuming experiments and allowed the authors to give some specific recommendations for perfecting the SHS extrusion process. (The recommendations are know-how and cannot be presented in this article.) Although this is very important, it is not the most important. The main thing is that theory together with experiment shapes the ideology of SHS extrusion. It should be emphasized that it is practical problems that stimulated theoretical studies.

There are many questions that could not be answered within the thermal theory presented here. In practice, qualitative and quantitative analyses of the stress-strain state of a material and of detailed blank volume distribution of density etc. are of primary importance. This required further complication of the thermal models presented here in order to include high-temperature deformation and compaction of porous bodies. Rheodynamic models were therefore formulated that reveal directly the role of rheological factors - volume and shear viscosities and their dependence on temperature and density. The results obtained using the rheodynamic models are reviewed in Part 2 of this article.

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