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MATHEMATICAL MODELLING OF DEFORMATION OF POROUS ORGANIC MATERIALS

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In this paper, we propose a method to describe the dynamics of deformation of polymeric materials under thermal and mechanical impacts. The method is based on solving the equation for a viscous incompressible fluid in the quasi-stationary approximation. This method is implemented for the case of simple compression of a cylindrical sample, the thickness of which is much less than its diameter. We construct dependencies of the viscosity coefficient on temperature and determine the relaxation time for the Maxwell mathematical model. It is shown that the viscosity of materials strongly depends on temperature, and this dependence is exponential. The performed calculations of the deformation of various polymeric materials demonstrate satisfactory agreement with the experimental data over the entire temperature range.

Keywords: viscous incompressible fluid; Maxwell mathematical model; heat conduction; equation of state.

Introduction

The problem on mathematical modelling of the behavior of porous organic materials under the action of mechanical and thermal loads is inextricably connected with the analysis and prediction of emergency situations that are caused by the use of energy materials in industry, their safe storage and operation. Accidents associated with fires in warehouses of energy materials occur quite regularly. Therefore, the relevant problems are safe handling of emergency products that fall into the thermal field of a fire, and a reliable assessment of the safe time spent by energy materials in the thermal field of a fire.

In products containing energy materials, there are parts from porous organic matter such as foam or penodiflon. This fact can significantly complicate such an assessment, since during heating, the parts can be significantly deformed as a result of thermal softening and mechanical action of the adjacent strong parts. The deformation, in turn, can lead to reducing thermal resistance (due to thinning and increased density) and reducing the predicted time before ignition. At present, an insufficient number of computational and theoretical studies of the behavior of thermoplastic materials under mechanical impact and elevated temperatures were carried out. For these purposes, it is necessary to develop a mathematical model of deformation, which should take into account thermal softening to correct the estimate of material deformation, as well as an increase in density (decrease in porosity) under force impacts and elevated temperatures.

In this regard, in this work, we carry out mathematical modelling of the behavior of thermoplastic materials under mechanical action in the temperature range 70°-180°C and compare the results obtained with the experimental data given in [1].

1. Mathematical Model of Deformation of Thermoplastic Materials

There exist viscous fluids that behave like solids for short time intervals, which are long compared to molecular times. Such amorphous solids can be considered as the limiting case of such viscous fluids.

The properties of such fluids can be described in terms of the Maxwell model [2]. For short periods of time, these fluids are elastically deformed. After the deformation stops, shift stresses remain in the fluids and decay with time. The stress decay time τ is called the Maxwellian relaxation time. At times of deformation much shorter than the relaxation time, the medium behaves like a solid body. At times of deformation of the order of time τ and more, the medium behaves like a fluid with a characteristic viscosity η

$$\eta \sim \mu\tau, \tag{1}$$

where μ is a shift modulus.

Experimental data on the deformation of thermoplastic materials under heating and mechanical load [1] very clearly demonstrate the properties of the materials under study as the properties of a very viscous fluid: at a constant load and temperature, the deformation process lasts for tens of minutes. At the initial moments of time after loading, according to the experimental data, an estimate of the medium flow velocity is $\sim 10^{-5}$ m/s, which is much less than the velocity of sound.

Thus, the deformation of thermoplastic materials can be described in terms of the model of a quasi-stationary flow of an incompressible fluid. The mathematical formulation of this model is expressed in the form of the incompressibility condition and the stationary Navier-Stokes equation:

$$(\nabla\vec{v}) = 0, \tag{2}$$

$$\rho\left(\vec{v}\nabla\right)\vec{v} = -\nabla P + \eta\nabla^2\vec{v}, \tag{3}$$

where ρ, P, $\vec{v}$ are mass density, pressure, velocity, respectively.

The geometry of the problem to be solved is shown in Fig. 1. A sample of material with the thickness h and the radius R is subjected to compression under the action of the force F, which is constant per unit area. During compression, the thickness of the sample decreases and, accordingly, its radius increases. We are interested in the dependence of the relative deformation of the sample on time:

$$\frac{\triangle\, h\left(t\right)}{h_0} = 1 - \frac{h\left(t\right)}{h_0}, \tag{4}$$

where h_0 is the thickness of the sample at the initial moment of time.

This problem is solved in a cylindrical coordinate system. The velocity field is characterized by the radial component $\upsilon_r\left(r,z\right)$ and the axial component $\upsilon_z\left(r,z\right)$. The boundary conditions on the velocity field have the following form:

a) the no-slip condition

$$\upsilon_r\left(r,z=0\right) = \upsilon_r\left(r,z=h\right) = 0 \tag{5}$$

is satisfied for the radial component of the velocity at the contact boundaries;

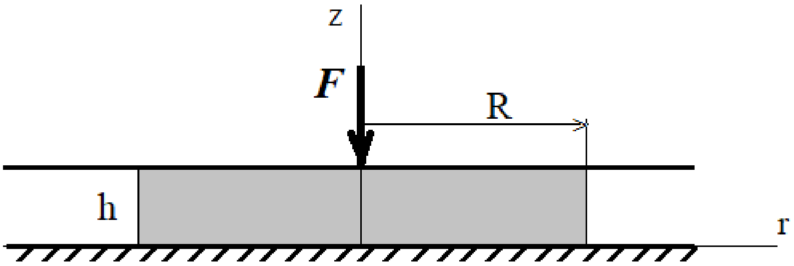

Fig. 1. Geometry of problem

b) for the axial velocity component, the condition is

$$v_z\left(r, z=0\right)=0, \quad v_z\left(r, z=h\right)=v_p, \tag{6}$$

where v_p is the velocity of movement of the upper plate of the press, which depends on the applied force F.

First of all, we take into account that the medium flow velocities are small ($\sim 10^{-5}$ m/s), which makes it possible to neglect the left side of equation (3), which contains the second powers of the velocity. In this case, the system of equations (2), (3) can be written as:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_r}{\partial r}\right)+\frac{\partial^2 v_r}{\partial z^2}=\frac{1}{\eta}\frac{\partial P}{\partial r}, \qquad \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)+\frac{\partial^2 v_z}{\partial z^2}=\frac{1}{\eta}\frac{\partial P}{\partial z}, \tag{7}$$

$$\frac{1}{r}\frac{\partial\left(r v_r\right)}{\partial r}+\frac{\partial v_z}{\partial z}=0. \tag{8}$$

At a given point in time, the sample thickness is defined as

$$h\left(t\right)=h_0-\int\limits_0^t v_z\left(h,t'\right)dt'. \tag{9}$$

Equations (7) – (9) with boundary conditions (5) and (6) form a system of equations that describe the quasi-stationary deformation of a sample under the action of the applied force.

In general case, the solution of this formulated system is possible only numerically, but for the case $h << R$ the system has a simple analytical solution similar to the solution obtained in [3]. To check the correctness of this approach to the description of the phenomenon under consideration, we use this analytical solution.

Since the medium is incompressible, its volume remains the same and is equal to $V_0=\pi R^2 h$. This implies:

$$\frac{v_p}{v_r\left(R\right)}=-\frac{2h}{R}, \tag{10}$$

where $v_p=\dot{h}$, $v_r\left(R\right)$ is the velocity of radial spreading of the sample during its compression, which is the maximum value in comparison with the velocities at other points of the medium.

It follows from (10) that the inequality $\upsilon_z << \upsilon_r$ holds for $h << R$. From the estimate of derivatives of velocities using expressions

$$\frac{\partial \upsilon_r}{\partial r} \sim \frac{\upsilon_r}{R}; \quad \frac{\partial \upsilon_r}{\partial z} \sim \frac{\upsilon_r}{h}; \quad \frac{\partial^2 \upsilon_r}{\partial r^2} \sim \frac{\upsilon_r}{R^2}; \quad \frac{\partial^2 \upsilon_r}{\partial z^2} \sim \frac{\upsilon_r}{h^2}, \tag{11}$$

we have

$$\frac{\partial \upsilon_r}{\partial r} << \frac{\partial \upsilon_r}{\partial z}; \quad \frac{\partial^2 \upsilon_r}{\partial r^2} << \frac{\partial^2 \upsilon_r}{\partial z^2}. \tag{12}$$

Of course, in expressions (12), the absolute values of the quantities are compared.

Taking into account (12), equations (7) take the form:

$$\frac{\partial^2 \upsilon_r}{\partial z^2} = \frac{1}{\eta}\frac{\partial P}{\partial r}; \qquad \frac{\partial P}{\partial z} = 0. \tag{13}$$

As follows from (13), the pressure is uniform along the depth of the sample, which allows us to represent the radial velocity component in the form:

$$\upsilon_r = \frac{1}{2\eta}\frac{\partial P}{\partial r} z\left(z - h\right). \tag{14}$$

From continuity equation (8) and solution (14) we find:

$$\upsilon_z = -\int_0^z \frac{1}{r}\frac{\partial\left(r\upsilon_r\right)}{\partial r}dz = -\frac{1}{2\eta r}\frac{\partial}{\partial r}\left[r\frac{\partial P}{\partial r}\left(\frac{z^3}{3} - \frac{hz^2}{2}\right)\right]. \tag{15}$$

Substituting boundary condition (6) into (15), we can find the pressure field in the compressible sample expressed in terms of the velocity of the upper press plate υ_p:

$$P\left(r\right) = \frac{3\eta\upsilon_p}{h^3}\left(R^2 - r^2\right) + P_0, \tag{16}$$

where P_0 is the external pressure. Using (16), it is easy to calculate the total force acting on the top plate of the press:

$$\pi R^2 F = 2\pi\int_0^R \left(P - P_0\right) r\,dr = \frac{3\pi\eta\upsilon_p R^4}{2h^3}. \tag{17}$$

From (17), we obtain the dependence of the press plate velocity on the applied force:

$$\upsilon_p\left(t\right) = \frac{2}{3}\frac{F}{\eta V_0}h^4\left(t\right). \tag{18}$$

Taking into account (9), expression (18) makes it possible to find the velocity υ_p, and, consequently, the fields of velocities, pressure, and deformation at any moment of time.

2. Numerical Research. Comparison with Experiment

The dynamics of deformation of thermoplastic materials at a given temperature and constant mechanical loading is calculated by formulas (4), (9) and (18). For calculations, expression (18) is represented as:

$$\upsilon_p\left(t_{n+1}\right)=\frac{2}{3}\frac{F}{\eta V_0}\left[h\left(t_n\right)-\upsilon_p\left(t_n\right)\vartriangle t\right]^4, \tag{19}$$

where $t_{n+1}=t_n+\vartriangle t$, $\vartriangle t$ is the time interval that is chosen so that the change in the medium flow velocity in this interval can be neglected. In the calculations below, the value of $\vartriangle t$ is $3-5$ s.

In (19), the unknown parameter is the relaxation time contained in expression (1), which is a function of temperature. At this stage of research, this value can be found only on the basis of experimental data. Since the spread of elastic constants for polymeric materials is quite large, then, instead of the relaxation time, we directly determine the viscosity coefficient on the basis of experimental data.

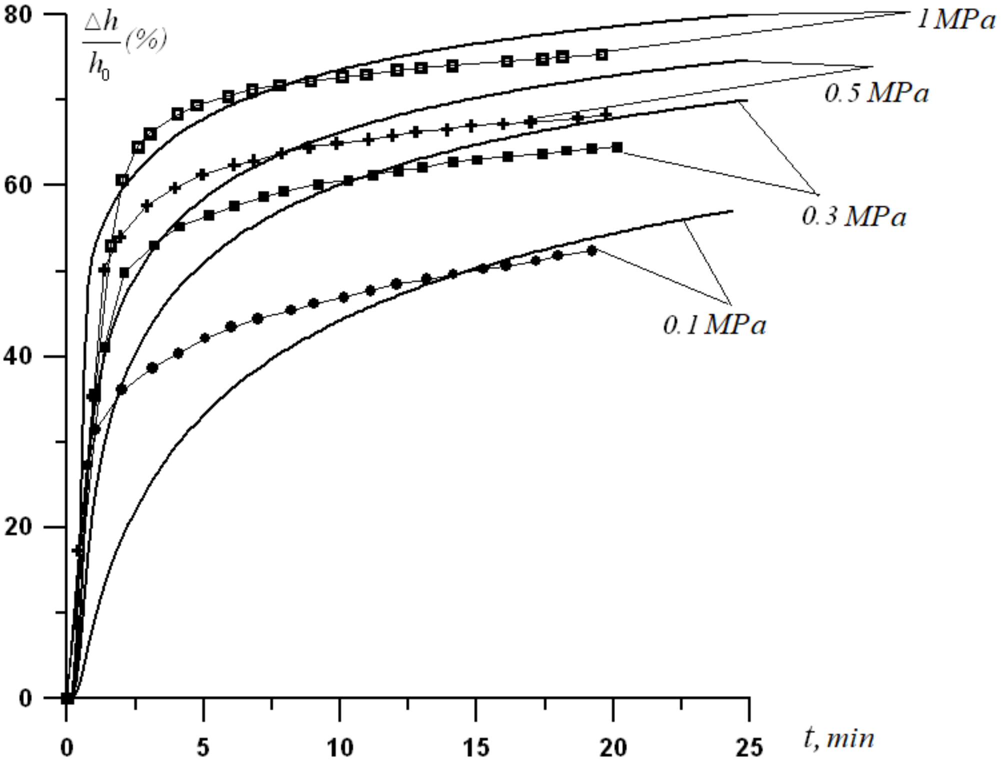

Fig. 2. Time dependence of relative deformation

Experimental data [1] are used to determine the viscosity coefficient. The calculations are carried out for a sample with the following parameters: the thickness is $h_0=7$ mm, the radius is $R_0=20$ mm. The pressures applied to the sample are set in the range $F=0.1-1.0\,\mathrm{MPa}$ $(1-10\,\mathrm{kgf/cm^2})$.

Fig. 2 shows the results of comparing the calculated and experimental dependencies of the relative deformation on time for the foam plastic PS-1, the polystyrene PS-1 at various

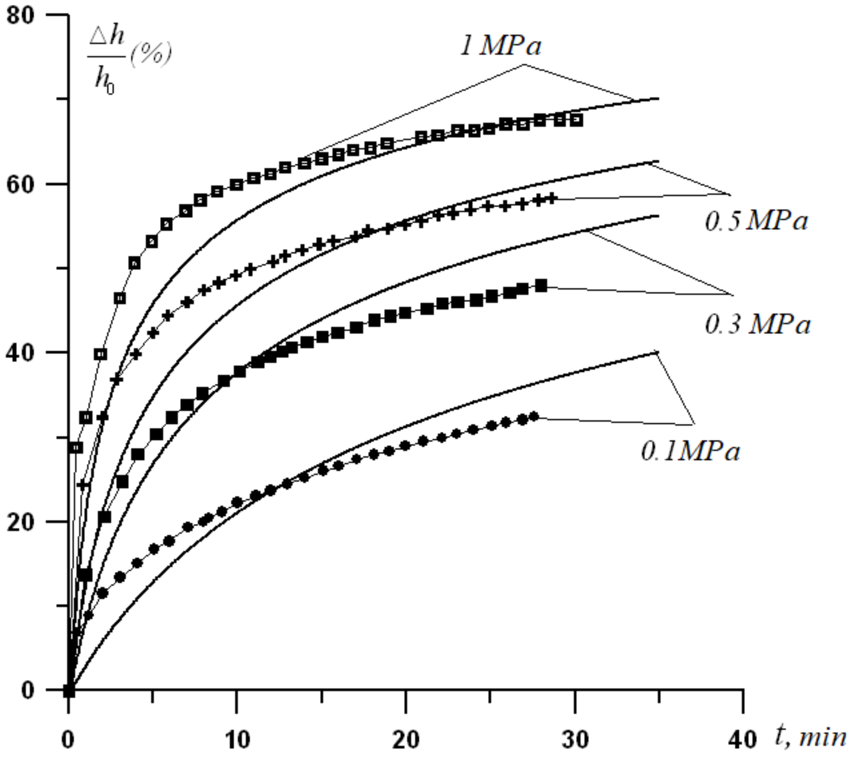

Fig. 3. Time dependence of relative deformation of ABS_2020

pressures and the temperature of 140°C. Markers denote experiment [1], lines represent calculations with the viscosity coefficient $\eta = 2 \cdot 10^6$ Pa·s.

The above comparisons indicate a qualitative agreement between the results obtained within the framework of the model considered here and the experimental data. The greatest discrepancy between the calculated and experimental results takes place at small deformations, which is primarily due to the non-fulfillment of the condition $h << R$ used in the model.

Similar calculations are carried out for the samples of the material ABS-2020 (Fig. 3). Markers denote experiment [1], lines represent calculations with the viscosity coefficient $\eta = 5.5 \cdot 10^6$ Pa·s. As in the previous calculations, the greatest discrepancy between the calculated and experimental results takes place at small deformations, that is, in the case when the condition $h << R$ is not satisfied.

Within the framework of this model, the values of the steady-state deformation of penodiflon at the temperature of 140 °C are also quite satisfactorily described at the value of the viscosity coefficient $\eta = 8 \cdot 10^8$ Pa·s. Comparisons of the calculated and experimental data are given in Tables 1–3. Tables 1–2 compare the steady-state values of relative deformations (at the time point of 30 minutes) with experimental data [1], as well as present the values of viscosity coefficients for various temperatures.

From the data given in Tables 1–3, it follows that with increasing sample temperature, the viscosity coefficient, and, consequently, the relaxation time, decrease, as a result of which the material becomes more fluid. It is noteworthy that for polystyrene there is an effect of «saturation» of viscosity: it remains constant in the range of 130° – 150 °C.

Fig. 4 shows the dependence of viscosity coefficients on temperature for various

Table 1

Relative deformation of the material foam plastic PS-1 at different temperatures and pressures

T°, C	$F = 0.1$ MPa Deformation %		$F = 0.3$ MPa Deformation %		$F = 0.5$ MPa Deformation %		$F = 1.0$ MPa Deformation %		Viscosity
	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Pa·s
95	14.1	15.4	30.5	30.3	37.1	38.1	47.3	48.9	$2.5\cdot10^7$
115	31.4	27.5	49.9	44.6	48.4	52.2	47.6	61.3	10^7
130	50.5	52.2	73.9	66.1	74.8	71.2	75.3	77.1	$2\cdot10^6$
140	52.5	52.2	64.1	66.1	68.2	71.2	75.1	77.1	$2\cdot10^6$
150	52.5	52.2	58.1	66.1	64.8	71.2	69.0	77.1	$2\cdot10^6$

Table 2

Relative deformation of the material ABS_2020 at different temperatures and pressures

T°, C	$F = 0.1$ MPa		$F = 0.3$ MPa		$F = 0.5$ MPa		$F = 1.0$ MPa		Viscosity
	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Pa·s
115	5.1	5.4	12.1	13.4	18.5	19.3	27.9	29.1	$9\cdot10^7$
140	32.1	36.8	47.6	53.3	58.3	60.0	67.7	68.1	$5.5\cdot10^6$
150	41.6	49.0	60.1	63.5	66.8	69.0	76.8	75.3	$2.5\cdot10^6$

Table 3

Relative deformation of the penodiflon material at different temperatures and pressures

T°, C	$F = 0.1$ MPa		$F = 0.3$ MPa		$F = 0.5$ MPa		$F = 1.0$ MPa		Viscosity
	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Pa·s
140	1.6	0.67	3.4	1.96	5.6	3.2	5.8	5.9	$8\cdot10^8$
150	7.2	6.72	15.2	16.0	20.9	22.6	34.9	33.0	$7\cdot10^7$
180	51.4	49.	69.5	63.0	71.9	69.0	75.2	75.3	$2.5\cdot10^6$

materials. It follows from the above dependencies that the viscosity of materials strongly depends on temperature, and this dependence is exponential – on a logarithmic scale, the dependencies on temperature are close to a linear law.

Based on the viscosity values found, the relaxation time can be estimated. The shift modulus of polystyrene is $\mu \sim 10^7$ Pa, which leads to the relaxation time $\tau = 0.2 - 2.5$ s. The ABS_2020 shift modulus is $\mu \sim 10^9$ Pa and then $\tau = 2.5 - 100$ ms.

3. Conclusions

Based on the results of this analysis, the following conclusions can be drawn.

1. The results presented in this paper show that for the case of simple compression of cylindrical samples of porous organic materials, the thickness of which is much less than its diameter, the properties of the material can be described in terms of the Maxwell model [2].

2. The performed calculations demonstrate satisfactory agreement with the

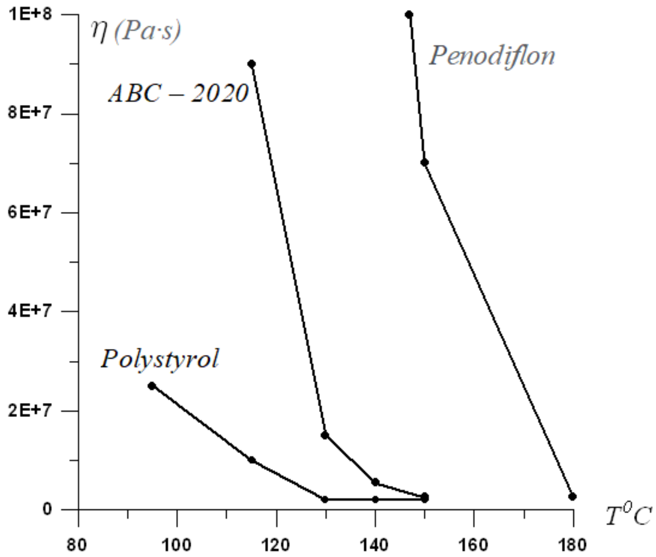

Fig. 4. Dependence of viscosity coefficients on temperature

experimental data. Based on the experimental data, an estimate of the relaxation time of the materials polystyrene PS-1 and ABS-2020 is obtained: for polystyrene, the relaxation time is 0.2 – 2.5 s in the temperature range 95° – 150° C, while for ABS_2020 the relaxation time is 2.5 – 100 ms in the temperature range 115° – 150° C.

3. To obtain more accurate data on the temperature dependence of the viscosity coefficients using this method, it is necessary to have a more detailed dependence of the relative deformation of samples on temperature than that presented in [1], taking into account the velocity of their heating. The latter circumstance is significant, especially at low temperatures, at which the relaxation time is especially long.

4. To apply the proposed model for describing the dynamics of deformation of polymeric materials under thermal and mechanical impacts in real structures, it is necessary to develop a method for solving equations in arbitrary geometry and arbitrary boundary conditions, taking into account real state equations [4, 5] of the material and methods for calculating the effective thermal conductivity [6].

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МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ДЕФОРМИРОВАНИЯ ПОРИСТЫХ ОРГАНИЧЕСКИХ МАТЕРИАЛОВ

А. А. Айдерханова, Ю. М. Ковалев, А. П. Яловец

В данной работе предложен метод описания динамики деформирования полимерных материалов при температурном и механическом воздействии. Метод основан на решении уравнения для вязкой несжимаемой жидкости в квазистационарном приближении. Данный метод реализован для случая простого сжатия цилиндрического образца, толщина которого много меньше его диаметра. Были построены зависимости коэффициента вязкости от температуры и определено время релаксации для математической модели Максвелла. Показано, что вязкость материалов сильно зависит от температуры, причем эта зависимость носит экспоненциальный характер. Проведенные расчеты деформирования различных полимерных материалов продемонстрировали удовлетворительное согласие с экспериментальными данными во всем диапазоне температур.

Ключевые слова: вязкая несжимаемая жидкость; математическая модель Максвелла; теплопроводность; уравнение состояния.

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