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Interrelations between heat and mechanical processes during solid phase chemical conversion under loading

A.G. Knyazeva a, N.K. Evstigneev b,*

 a Institute of Strength Physics and Materials Science SB RAS, 2/4, Akademicheskii pr., Tomsk, 634055, Russia
 b Tomsk State University, 36, Lenina pr., Tomsk, 634050, Russia

Abstract

The mathematical model of solid-phase chemical reaction propagation in a plate under mechanical loading is suggested. Uniaxial tension, shearing and anchorage of the plate edges are considered. The problem is solved in two-dimensional definition. Parametric investigation of the model is carried out. Stress and strain field evolution is investigated. Influence of coupling between the fields of temperature, concentration and stress on the chemical conversion propagation is illustrated.

Keywords: stress; strain; uniaxial tension; shearing; anchorage; solid-phase chemical reaction.

1. Introduction and physical problem definition

Initiation of a chemical conversion in a solid body by external action always leads to stress field appearance. The reasons of it are different: nonuniformity of matter heating, inhomogeneity of matter structure, differences between specific volumes of reactants and reaction products or mismatch of their structure and so on. Thus if an external source is a thermal one, some part of heat is spent on deformation which leads to heating-up delaying and reducing the reaction rate. If external source is a mechanical impulse, then relaxation of stresses besides matter destruction and generation of structure defects is accompanied by the heat release. Both effects follow from coupling of temperature and strain fields. One of the ways which let us change combustion properties and regulate the structure of reaction products is the action of constant load on gas-free mixture burning in mold. The load may determine process behavior, hasten or decelerate the conversion, change the kinetics of structure formation processes. Influence of stresses on the rate of elastically strained bonds rupture reaction, \( k \), is described by Eyring-Kozman equation [1]

\[
k = k_0 \exp \left( -\frac{E_a - \sigma V}{RT} \right).
\]

* Corresponding author. Tel.: +7-913-847-89-47.
E-mail address: evstigneev.nk@rambler.ru.

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Here \( k_0 \) and \( E_a \) are the pre-exponential factor and the energy of thermal decomposition activation, \( \sigma V_a \) – the work of elastic stresses (\( \sigma \) is stress, \( V_a \) is activation volume), \( R \) is the universal gas constant, \( T \) is the temperature. It is implied that the action of stresses facilitates energy barrier passage but does not influence its height. Such approximation seems to be correct in elastic area and \( \sigma \) means local stresses.

Investigations of solid-phase chemical conversions under mechanical loading started several decades ago. Such authors as O.B. Kovalev, V.V. Boldyrev, N.S. Enikolopyan and some others made a considerable contribution to this field of science, but most of their works are experimental ones. And still there is a lack of mathematical models describing these processes. No models taking into account coupling effect in chemical transformations were found in publications.

The present paper presents the model of solid-phase chemical reaction under mechanical loading which takes into account variation of conversion rate because of the action of stresses. Two types of external loading are considered: uniaxial tension and shearing. Besides that, the anchorage of plate edges was also investigated. Kinetics equation takes into account the fact that there are two main ways of chemical reaction initiation: changing internal energy (temperature) and producing work. Thus the function of chemical heat release takes the form

\[
\phi(Y,T) = k_0(1-Y)\exp\left(-\frac{E_a - k_1\Pi}{RT}\right)
\]

where \( Y \) is the conversion degree, i.e., the concentration of reaction product, \( k_1 \) is the coefficient of reaction rate sensitivity to the work of stresses, \( \Pi = -\sum_{\langle ij \rangle \neq \langle x,y,z \rangle} \sigma_{ij} \varepsilon_{ij} \) is the work of stresses, \( \sigma_{ij} \) – stress tensor components, \( \varepsilon_{ij} \) – strain tensor components.

If stress tensor is a spherical one, then

\[
\Pi = -[\sigma_{xx}\varepsilon_{xx} + \sigma_{yy}\varepsilon_{yy} + \sigma_{zz}\varepsilon_{zz}] = -\sigma_{xx}\varepsilon_{xx} = \frac{P}{3} \varepsilon_{xx}.
\]

In such case \( k_0 \) may be connected with the activation volume: \( k_0 = V_a \Delta \gamma_m \), where \( \gamma_m \) is the local molar volume.
Fig. 1. illustrates the problem definition. It is supposed that the sample is a stationary thin plate from a reactive material. The plate length \( L_x \), the width is \( L_y \), and the height \( L_z \) is much less than \( L_x \) and \( L_y \). In case of uniaxial tension the distributed loading of the value \( \sigma_{xx} = P \) is applied to the plate faces \( x = 0 \) and \( x = L_x \). The direction of the load coincides with \( Ox \) axis. In case of shearing loading \( \sigma_{xy} = P \) is applied to the plate perimeter. In case of the plate anchorage all its edges are fixed.

Exothermic chemical reaction which may be described with a simple total scheme \( A \rightarrow B \) spreads in the direction of \( Ox \) axis. It is considered that the melting temperature is not reached and the whole reaction progresses in a solid phase. Such requirement is a necessary condition of some materials synthesis technologies. As far as the mechanical disturbances propagation velocity is much greater than the solid-phase chemical reaction propagation rate, inertial forces were neglected in the first approximation. Heat exchange with the environment was not taken into account. Mechanical moduluses of the material \((E, \mu)\) are considered to be constant during the whole process.

2. Mathematical problem definition and nomenclature

As far as \( L_z \) is much less than \( L_x \) and \( L_y \), let’s proceed to the generalized plane stress approximation [2]. In such case the system of stress equilibrium equations takes the form

\[
\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0, \tag{1}
\]

\[
\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0. \tag{2}
\]

We have only one strain compatibility condition:

\[
\frac{\partial^2 \varepsilon_{xx}}{\partial y^2} + \frac{\partial^2 \varepsilon_{yy}}{\partial x^2} = \frac{\partial^2 \varepsilon_{xy}}{\partial x \partial y}. \tag{3}
\]

Relationship between the stress and strain tensor components is expressed with the generalized Duhamel-Neumann one [3]

\[
\varepsilon_{xx} = \frac{1}{E} (\sigma_{xx} - \mu \sigma_{yy}) + \frac{\omega}{3}, \tag{4}
\]

\[
\varepsilon_{yy} = \frac{1}{E} (\sigma_{yy} - \mu \sigma_{xx}) + \frac{\omega}{3}, \tag{5}
\]

\[
\varepsilon_{xy} = \frac{2(1 + \mu)}{E} \sigma_{xy}, \tag{6}
\]

where \( \omega = \frac{3}{2} \left[ \alpha_r (T - T_0) + (\alpha_r - \alpha_e) Y \right] \) is the function of volume expansion, \( \alpha_r \) is the coefficient of heat expansion, \( \alpha_p \) and \( \alpha_e \) are the coefficients of structural expansion of reaction product and reagent respectively, \( E \) is the modulus of elasticity, \( \mu \) is the Poisson ratio.

Differentiating (1) and (2) with respect to \( x \) and \( y \) and substituting the result together with (4)–(6) into (3), we get the system of equations to determine nonzero components of the stress tensor:

\[
\Delta \sigma_{xx} = -\frac{E}{3} \Delta \omega, \]

\[
\Delta \sigma_{yy} = \frac{\partial^2 \sigma_{xx}}{\partial x^2},
\]
\[ \Delta \sigma_{\nu} = \frac{\partial^2 \sigma_{\nu}}{\partial x \partial y}, \]

where \( \Delta \) is the Laplace operator and \( \sigma_{\nu} = \sigma_{xx} + \sigma_{yy} \).

In case of the plate anchorage it is more convenient to use the displacement equations:

\[
\begin{align*}
\frac{\partial^2 u}{\partial x^2} + \frac{1 - \mu}{2} \frac{\partial^2 u}{\partial y^2} + \frac{1 + \mu}{2} \frac{\partial^2 v}{\partial x \partial y} - \frac{1 + \mu}{3} \frac{\partial \omega}{\partial x} &= 0, \\
\frac{\partial^2 v}{\partial y^2} + \frac{1 - \mu}{2} \frac{\partial^2 v}{\partial x^2} + \frac{1 + \mu}{2} \frac{\partial^2 u}{\partial x \partial y} - \frac{1 + \mu}{3} \frac{\partial \omega}{\partial y} &= 0.
\end{align*}
\]

Using the dimensionless variables

\[ s_y = \frac{\sigma_y}{\sigma_x}, \quad e_y = \frac{e_y}{e_x}, \quad \bar{u} = u, \quad \bar{v} = v, \quad \xi = \frac{x}{x_c}, \quad \eta = \frac{y}{y_c}, \quad \bar{\omega} = \frac{\omega}{\omega_x}. \]

where \( \sigma_x = 3K\alpha_\tau(T_\tau - T_0), \quad e_x = \omega_x = 3\alpha_\tau(T_\tau - T_0), \quad x_c = y_c = \frac{\lambda_\tau T_\tau}{c \rho}, \quad u_c = \omega_x, \quad t_c = \frac{c \rho RT_c^2}{E_x Q_k}, \quad T_\tau = T_\tau + \frac{Q}{c \rho}, \quad K \) is the compression modulus,

we get stress equations for the uniaxial tension and shearing

\[ \Delta s_{xx} = (2\mu - 1)\Delta \bar{\omega}, \quad (7) \]
\[ \Delta s_{yy} = \frac{\partial^2 s_{yy}}{\partial \xi^2}, \quad (8) \]
\[ \Delta s_{xy} = -\frac{\partial^2 s_{xy}}{\partial \xi \partial \eta}, \quad (9) \]

and the displacement equations for the plate anchorage

\[
\begin{align*}
\frac{\partial^2 \bar{u}}{\partial \xi^2} + \frac{1 - \mu}{2} \frac{\partial^2 \bar{u}}{\partial \eta^2} + \frac{1 + \mu}{2} \frac{\partial^2 \bar{v}}{\partial \xi \partial \eta} - \frac{1 + \mu}{3} \frac{\partial \bar{\omega}}{\partial \xi} &= 0, \\
\frac{\partial^2 \bar{v}}{\partial \eta^2} + \frac{1 - \mu}{2} \frac{\partial^2 \bar{v}}{\partial \xi^2} + \frac{1 + \mu}{2} \frac{\partial^2 \bar{u}}{\partial \xi \partial \eta} - \frac{1 + \mu}{3} \frac{\partial \bar{\omega}}{\partial \eta} &= 0.
\end{align*}
\]

Stress boundary conditions in case of uniaxial tension are of the form

\[ \xi = 0, \quad \xi = L_\xi: \quad s_{xx} = \bar{P}, \quad s_{yy} = 0, \quad s_{xy} = 0, \]
\[ \eta = 0, \quad \eta = L_\eta: \quad s_{xx} = 0, \quad s_{yy} = 0, \quad s_{xy} = \bar{P}. \]

in case of shearing look like

\[ \xi = 0, \quad \xi = L_\xi: \quad s_{yy} = 0, \quad s_{xx} = 0, \quad s_{xy} = \bar{P}. \]
\[ \eta = 0, \quad \eta = L_\eta : \quad s_{u\eta} = 0, \quad s_{\eta\eta} = 0, \quad s_{u\eta} = \overline{P}, \]

and for the plate anchorage take the form

\[ \xi = 0, \quad \xi = L_\xi : \quad \overline{u} = 0, \quad \overline{v} = 0, \]

\[ \eta = 0, \quad \eta = L_\eta : \quad \overline{u} = 0, \quad \overline{v} = 0. \]

Here \( \overline{P} = \frac{P}{3\kappa\alpha_r(T_r - T_0)} \) is the dimensionless value of external load.

Chemical reaction propagation problem in dimensionless variables

\[ \theta = \frac{T - T_u}{T_r - T_u}, \quad \tau = \frac{t}{t_r}, \]

takes the form

\[ \frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial \xi^2} + \frac{\partial^2 \theta}{\partial \eta^2} + \frac{\partial Y}{\partial \tau} - \delta(\theta + \sigma_r) \frac{\partial e_u}{\partial \tau}, \tag{12} \]

\[ \frac{\partial Y}{\partial \tau} = \frac{1}{\theta_0}(1 - Y) \exp \left( \frac{\theta - 1 - \delta \Lambda(\sigma_r + 1) \sum s_i e_i}{\beta(\theta + \sigma_r)} \right), \tag{13} \]

\[ \overline{\omega} = \theta + g \cdot Y. \]

Starting and boundary conditions we’ll write as:

\[ \tau = 0 : \quad \theta = 0, \quad Y = 0, \]

\[ \xi = 0 : \quad \frac{\partial \theta}{\partial \xi} = \overline{q}_0, \quad \xi = L_\xi : \quad \frac{\partial \theta}{\partial \xi} = 0, \]

\[ \eta = 0 : \quad \frac{\partial \theta}{\partial \eta} = 0, \quad \eta = L_\eta : \quad \frac{\partial \theta}{\partial \eta} = 0. \]

Dimensionless parameters are as follows: \( \delta = \frac{\kappa \alpha_x \omega_x}{c \rho} \), \( \sigma_r = \frac{T_r}{T_r - T_0} \), \( \theta_0 = \frac{1}{\beta(\theta + \sigma_r)} \), \( A = \frac{k_e Q}{E} \), \( \beta = \frac{RT}{E} \),

\[
g = \frac{\alpha_y - \alpha_x}{\alpha_x (T_r - T_0)} \quad \overline{q}_0 = \frac{q_{0\chi}}{\kappa \chi (T_r - T_0)} \quad L_\xi = \frac{L_x}{x} \quad L_\eta = \frac{L_y}{y}.\]
Physical interpretation of these values is as follows: \( \delta \) – the coefficient of coupling between heat transfer and deformation processes, \( \sigma_T \) – the ratio of initial temperature to heat warming up, \( \theta_0 \) – Zel’dovich number, \( A \) – the coefficient of reaction rate sensitivity to the work of stresses, \( \beta \) – the small parameter, characterizing reaction rate sensitivity to temperature, \( g \) – relative volume change in the process of chemical conversion (ratio of concentration deformation to the thermal one), \( \eta_0 \) – external heat flux intensity; \( L_z \) – dimensionless plate length, \( L_\eta \) – dimensionless plate width.

Notation conventions: \( \lambda_T \) – heat conductivity factor, \( c \) – heat capacity, \( \rho \) – density (in the general case all physical properties depend on porosity), \( Q \) – thermal effect of chemical reaction, \( q_0 \) – heat flow density. “0” index denotes initial conditions.

3. Computation results and discussion

Problem was solved numerically. Equations (7)–(11) were solved using the successive over-relaxation method [4]. The finite-difference scheme for Poisson equation

\[
\frac{\partial^2 F}{\partial z^2} + \frac{\partial^2 F}{\partial \eta^2} = \phi(\xi, \eta)
\]

takes the form

\[
F_{i,j}^{k+1} = F_{i,j}^k + \frac{W_0}{2(1+\gamma^2)}[F_{i,j}^k + F_{i,j-1}^{k+1} + \gamma^2 F_{i,j-1}^{k} + \gamma^2 F_{i-1,j}^{k+1} - \Delta \xi^2 \phi_{i,j} - 2(1+\gamma^2)F_{i,j}^k],
\]

where \( k \) is the number of iterations, \( W_0 \) is the relaxation parameter, \( \gamma = \Delta \xi / \Delta \eta \).

Heat conduction equation (12) was solved with the help of the alternating direction method [5]. The finite-difference scheme for the equation

\[
\frac{\partial F}{\partial t} = \frac{\partial^2 F}{\partial z^2} + \frac{\partial^2 F}{\partial \eta^2} + \phi(\xi, \eta)
\]

may be written as

\[
\frac{F_{i,j}^{n+1/2} - F_{i,j}^n}{\Delta t / 2} = \frac{F_{i,j}^{n+1/2} - 2F_{i,j}^{n+1/2} + F_{i,j}^{n+1/2}}{\Delta \xi^2} + \frac{F_{i,j}^n - 2F_{i,j+1}^n + F_{i,j+1}^n}{\Delta \eta^2} + \phi_{i,j}^n,
\]

\[
\frac{F_{i,j}^{n+1/2} - F_{i,j}^{n+1/2}}{\Delta t / 2} = \frac{F_{i,j}^{n+1/2} - 2F_{i,j}^{n+1/2} + F_{i,j}^{n+1/2}}{\Delta \xi^2} + \frac{F_{i,j}^{n} - 2F_{i,j+1}^{n} + F_{i,j+1}^{n}}{\Delta \eta^2} + \phi_{i,j}^n.
\]

Here \( n \) is the number of the time layer. Sweep method was used for solving the system of finite-difference equations.

Equation (13) was resolved using the explicit-implicit difference scheme. Within the scope of \( Y \) variable the scheme is implicit, and temperature and stress and strain tensor components are calculated beforehand within the same time step:

\[
\frac{Y_{i,j}^{n+1} - Y_{i,j}^n}{\Delta t} = \frac{1}{\theta_0} (1 - \xi_{i,j}^{n+1}) \exp \left( \frac{\theta_{i,j}^{n+1} - 1 - \delta \lambda (\sigma_{i,j} + 1)(s_{i,j} e_{i,j}^* + s_{i,j} e_{i,j}^*)}{\beta (\theta_{i,j}^{n+1} + \sigma_{i,j})} \right).
\]

Plate size is \( 10 \times 10 \) sm. Estimated parameters were calculated on the basis of reference data for Ti+Ni system. Varying \( T \) from 900 to 1200 °C we obtain \( 0.3 < \sigma_T < 0.23, 0.09 < \beta < 0.12 \). The value of coefficient of reaction rate
sensitivity to the work of stresses depends on matter type and should be defined experimentally. In the calculations it was fixed that \( \sigma_t=0.25, \beta=0.1, L_\xi=15, L_\eta=15, \nu=0.33. \) \( A, \delta, g, \bar{P} \) parameters were varied widely: \( A=0\ldots20, \delta=0\ldots0.06, g=-1.5\ldots1.5, \bar{P} = 0\ldots2 \).

Program was tested:
1) Calculation was made for the next extreme case: inert problem without external load and without chemical reaction, \( L_\xi\to\infty. \) In such case equation (12) has exact analytical solution

\[
0(\xi,\eta,\tau) = 2q \sqrt{\frac{\tau}{\pi}} \cdot \exp\left( -\frac{\xi^2}{4\tau} \right) - q\xi \cdot \text{erfc}\left( \frac{\xi}{2\sqrt{\tau}} \right),
\]

which was reproduced numerically accurate within 1 %.

2) Temperature is constant, no chemical reaction. In case of uniaxial tension maximum stress values ( \( s_{\eta} = \bar{P} \) ) are located on loading surfaces and decrease deep into the plate, stress field is symmetrical with respect to line \( \eta=L_\eta/2. \)

After program testing the distributions of temperature, conversion degree, stress and strain tensor components in various points of time were calculated; surface temperature evolution, mean conversion degree and chemical reaction propagation velocity were analyzed in the course of numerical investigation of the problem.

Maximum temperature during the whole process was obtained on the plate surface \( \xi=0. \) Increase of the coefficient of reaction rate sensitivity to the work of stresses leads to its insignificant growth in the beginning of the process. In case of uniaxial tension the temperature maximum is formed on the plate’s axis of symmetry \( \eta=L_\eta/2 \) with the course of time, and in case of shearing the maximum temperature point migrates along the line \( \xi=0 \) in the direction of greater values of \( \eta \) during the process. It is caused by the influence of stress work and the fact that in case of shearing there is no axis of symmetry.

Let’s consider the mean conversion degree: \( \langle Y \rangle = \frac{1}{L_\xi L_\eta} \int_0^{L_\eta} \int_0^{L_\xi} Y d\xi d\eta. \)

![Fig. 2. Influence of the sensitivity coefficient on chemical conversion in case of uniaxial tension (a) and shearing (b). \( \sigma_t=0.25, \beta=0.1, L_\xi=15, L_\eta=15, g=0.5, \bar{P} = 1, \bar{q}_0 = 0.5, A=10, 1 – \delta=0, 2 – \delta=0.03, 3 – \delta=0.06. \)](image1)

Fig. 2 shows that taking into account the coupling effect under loading conditions might substantially amend process dynamics. Comparing curves 1 and 3, one can see that half reaction time experiences twofold variation if we change \( \delta \) from 0 to 0.06. In case of plate anchorage the influence of the sensitivity coefficient is insignificant and it is not shown on figure 2.
Comparing the curves on fig. 2 one can see that shearing as the type of external load leads to more rapid chemical conversion in regard to uniaxial tension, which is detected in many experimental researches. One should expect greater effect using the models which take into account dynamic phenomena.

Fig. 3. Evolution of the stress tensor (a-c) and strain tensor (d-f) first invariants in case of uniaxial tension. $\tau=5$ (a, d), $\tau=15$ (b, e), $\tau=30$ (c, f). $\sigma=0.25$, $\beta=0.1$, $L_{\xi}=15$, $L_{\eta}=15$, $g=0.5$, $\bar{P}=1$, $\bar{q}=0.5$, $A=10$, $\delta=0.03$.

Fig. 3 shows the evolution of stress and strain tensors’ first invariants in case of uniaxial tension. Bending of stress isolines on fig. 3, b, c gives us the information on reaction front position: $\xi=2$ at $\tau=15$ and $\xi=5$ at $\tau=30$, which is confirmed by comparison with concentration field (fig. 4, e, f). With the help of fig. 3 one can see the plate deformation growth.

Fig. 4. Evolution of the temperature (a-c) and the conversion degree (d-f) fields in case of uniaxial tension. $\tau=5$ (a, d), $\tau=15$ (b, e), $\tau=30$ (c, f). $\sigma=0.25$, $\beta=0.1$, $L_{\xi}=15$, $L_{\eta}=15$, $g=0.5$, $\bar{P}=1$, $\bar{q}=0.5$, $A=10$, $\delta=0.03$. 
We’d like to note that the deformations caused by the chemical reaction reach large values and substantially exceed the deformations caused by external loading. If there is no chemical reaction then the maximum value of strain tensor invariant is $\varepsilon_k=0.45$, after the conversion in hot area we get $\varepsilon_k=4.49$.

Different ways of loading lead to the fact that the flame front spreads not as a stripe parallel to $\eta$ axis, but bends according to the way of loading. Thus in case of uniaxial tension $Y(\xi, \eta)$ and $\theta(\xi, \eta)$ isolines are symmetrical with respect to the line $\eta=L_\eta/2$ (fig. 4). Under more complicated loading – shearing – the symmetry breaks. Such is the picture for all the components of stress and strain tensors.

It seems to be interesting for the qualitative analysis of the process dynamics to make an equivalent “sigma-epsilon” chart for area-average values of first invariants of stress and strain tensor components:

$$\langle s_{\alpha\alpha} \rangle = \frac{1}{L_x L_\eta} \int_0^{L_x} \int_0^{L_\eta} s_{\alpha\alpha} d\xi d\eta, \quad \langle e_{\alpha\alpha} \rangle = \frac{1}{L_x L_\eta} \int_0^{L_x} \int_0^{L_\eta} e_{\alpha\alpha} d\xi d\eta.$$  

Fig. 5. “Sigma-epsilon” chart in case of uniaxial tension (a), shearing (b) and anchorage (c). $1 - \delta = 0, A = 0, 2 - \delta = 0.03, A = 0, 3 - \delta = 0.03, A = 10, 4 - \delta = 0.03, A = 20$. $\sigma_r=0.25, \beta=0.1, L_\xi=15, L_\eta=15, g=0.5, \overline{P} = 1, \overline{q}_0 = 0.5$.

As follows from fig. 5, in case of the plate anchorage neither taking into account the coupling effect, nor varying the sensitivity coefficient can influence the chart. But for other types of loading such influence is essential.

Parameter $g$, which characterizes the volume change during the conversion, has a strong effect on process dynamics. If $g>0$, the conversion progresses with volume expansion, if $g<0$ – with volume contraction.

Fig. 6 shows changing of “sigma-epsilon” charts according to different values of parameter $g$.

It was found out that varying the parameter which is related to chemical reaction, it is possible to obtain qualitatively different dependencies between mean stresses and mean strains. Thus if $g<0$ curve 3 resembles creep curve though the problem was solved within the scope of elastic statement.
4. Conclusion

Two-dimensional mathematical model describing the influence of various types of external loading on the solid-phase chemical conversion in a plate was suggested. The model takes into account interrelations between the mechanical stresses and the chemical conversion (heat release in reaction and differences between specific volumes of reagent and reaction product). The algorithm of numerical investigation of the model was developed. Parametric investigation of the model was carried out. It was found out that the stresses and strains appearing in the process of conversion play an important role in the dynamics of the process. The influence of loading conditions on chemical conversion in the plate was shown. The model is to be updated. The authors are going to work further on taking into account dependences of physical properties on the temperature and conversion degree. Another area of work will include introducing more complicated chemical kinetics. The ideas of the work will be developed and used for simulation of SHS-extrusion of intermetallic compounds.

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