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Modeling of Solid Propellants Viscoplastic Behavior Using Evolutionary Algorithms

Robert ZALEWSKI[1*], Mariusz PYRZ[2]
and Tomasz WOLSZAKIEWICZ[3]

[1] *Institute of Machines Design Fundamentals, Warsaw University of Technology, 84 Narbutta St., 02-524 Warsaw, Poland*
[2] *Institute of Vehicles, Warsaw University of Technology, 1 Politechniki Sq., 00-661 Warsaw, Poland*
[3] *Institute of Industrial Organic Chemistry, Annopol 6, 03-236 Warsaw, Poland*
[*] *E-mail: robertzalewski@wp.pl*

Abstract: In the paper an initial attempt to the experimental analysis of viscous effects, characteristic for homogeneous solid rocket fuels is proposed. For this reason uniaxial tensile experiments, carried out on dumbbell homogeneous solid propellants have been chosen. Laboratory tests have been carried out on INSTRON tensile testing machine. Research schedule involved destructive tensile tests with various strain rates. Three different values of strain rates have been taken into consideration. Experimentally obtained hardening curves are presented in suitable diagrams.

Basing on obtained results, authors confirm the viscoplastic behavior of studied materials. Essential impact of the applied strain rate on the position of experimental hardening curves is observed. Acquired results are the base for the further stage of investigations of homogeneous solid propellants – the modeling of their physical properties.

Additionally, numerical modeling of studied phenomena, using the viscoplastic Chaboche's model, identified on the basis of experimental data, is presented. The material parameters of the constitutive law are determined numerically using an evolutionary algorithm procedure. The efficiency of the model and the identification approach are discussed.

Keywords: solid rocket fuel, experimental studies, modeling, constitutive law, evolutionary algorithms, numerical simulation

Introduction

To increase the operational safety of special objects, working on the basis of solid rocket fuels, also to improve their durability on aggressive working conditions, it is necessary to understand the complex physical features of energetic materials. Such materials, besides providing appropriate ballistic conditions, should be resistant to high temperatures and former mechanical (or thermal) loading history. Complex working conditions are connected to a particularly aggressive working environment, a frictional wear of solid propellants and a degradation of mechanical properties, caused by different external conditions.

Typical solid propellant consists of numerous chemical ingredients such as oxidizer, fuel, stabilizer, plasticizer, binder, curing agent, and cross-linking agent. The detailed chemical composition strongly depends on the desired combustion characteristics for a specific application. Two main types of propellants (heterogeneous and homogeneous) are distinguished by the condition in which their constituent ingredients are interconnected. In the first group of the previously mentioned materials, the ingredients are linked chemically and the resulting physical structure is homogeneous throughout. Typical examples of homogeneous propellants are single-base (NC nitrocellulose) or double-base (NC and NG nitroglycerine) propellants. In a heterogeneous or composite propellant, the ingredients are physically mixed, leading to a heterogeneous physical nature. It is mainly composed of crystalline oxidizers and organic plastic fuels acting as binder [1].

In this paper authors restricted themselves only to experimental tests carried out on typical homogeneous materials. All experimental tests have been carried out in the Laboratory of Energetic Materials of the Institute of Industrial Organic Chemistry (Warsaw, Poland).

Classical experimental methods applied in solid propellants are similar, from the mechanical point of view, to experimental methods of solid materials or plastics [2]. Generally, they are restricted to the most popular uniaxial experiments, mainly due to economical limitations. The tests are realized on standard tensile testing machines. Typical mechanical parameters, examined during laboratory tests, are Young modulus, Poisson ratio, tensile strength or yield limit [3].

Generally for solid bodies, viscoplasticity is the global behavior caused by a mechanism corresponding to the movement of dislocations in grains, with superposed effects of inter-crystalline gliding. This phenomenon mainly becomes principal at temperatures approximate to one third of the absolute melting temperature. However, some structural materials reveal viscoplasticity effects at room temperature. For plastics, wood, and bitumen, the theory of viscoplasticity is required to describe behavior beyond the limit of elasticity or viscoelasticity.

In general, viscoplasticity theories are useful in areas such as

- the calculation of permanent deformations,
- the prediction of the plastic collapse of structures,
- the investigation of stability,
- crash simulations,
- systems exposed to high temperatures such as turbines in engines, e.g. a power plant,
- dynamic problems and systems exposed to high strain rates.

As it was mentioned earlier, solid propellants are subjected to various external conditions very often strictly related to previously listed conditions.

To provide a suitable constitutive model for solid propellants, a lot of fundamental experiments have to be carried out. It is particularly interesting, that general standards for conducting basic strength properties experimental tests have not yet been elaborated for this class of materials. Such problems as quasi-static strain range for solid propellants or shape and dimensions of simple testing specimen are still not normalized. Also, the available data concerning the basic rheological properties of solid rocket fuels is insufficient. Though, this paper is the next stage of the preliminary investigation devoted to modeling of nonlinear properties of solid propellants.

Objectives and scope of the paper

The main objective of the paper is to study some experimental results confirming the viscoplastic like behavior of homogeneous solid propellants and to propose the numerical modeling of the phenomenon under investigation.

Basing on obtained results, authors confirm the viscoplastic behavior of considered materials. Essential impact of the applied strain rate on the position of experimental hardening curves is observed. Acquired results are the base for the further stage of investigations of homogeneous solid propellants – the choice of appropriate model for simulation of their physical properties. The global aim is to define a suitable constitutive law for the solid fuel material.

Numerical modeling, presented in the paper, applies the viscoplastic Chaboche's model. The material parameters of the constitutive law are determined numerically basing on the experimental data and using the evolutionary algorithm procedure. Uniaxial tensile tests, carried out on specially prepared samples, and studied for three various strain rates, are discussed. The efficiency of the model and the identification approach are discussed.

Experiments

To reveal the viscoplastic like behavior, universal tensile tests, on dumbbell homogeneous solid propellants samples (Figure 1) have been conducted. Three various strain rates values: 0.02 = 2 x 10^{-2} [1/s]; 0.002 = 2 x 10^{-3} [1/s] and 0.0002 = 2 x 10^{-4} [1/s], have been taken into consideration. The shape and dimensions of a testing sample are shown in Figure 1.

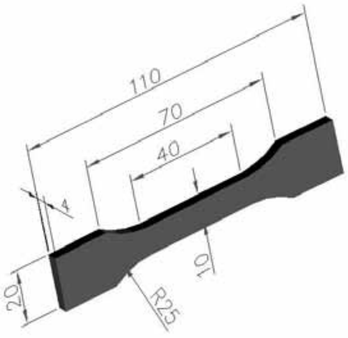

Figure 1. Experimental sample.

Experimentally acquired hardening curves are depicted in Figure 2.

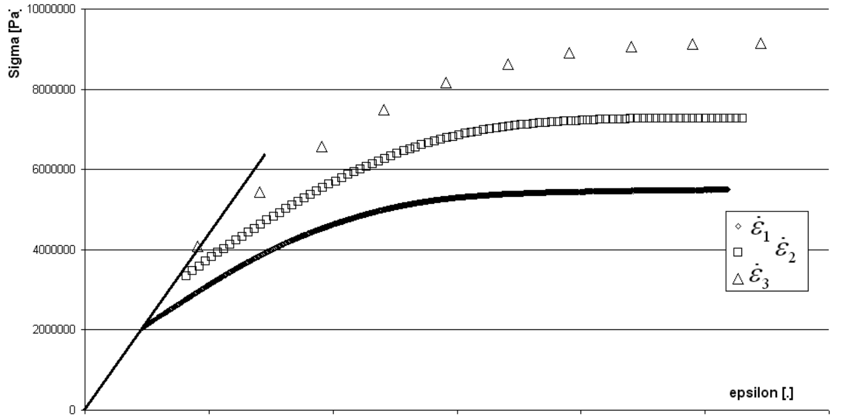

Figure 2. Experimental data for various strain rates.

To compare obtained data for both experimental specimens, direct experimental records (force [N], elongation [mm] and time [s]) have been transformed into stress [Pa] and an engineering strain [.], using formulae (1) and (2):

$$\sigma = \frac{F}{ab}, \qquad (1),$$

$$\varepsilon = \frac{l - l_0}{l}, \qquad (2)$$

where: *a,b* are cross-section dimensions of the gauge length of the testing piece, *F* – tensile force [N], l_0, *l* – original and temporary gauge length of a testing specimen respectively.

Basing on results illustrated in Figure 2, typical viscoplastic like behavior of considered samples have been noticed. The higher strain rate corresponds to higher position of the experimentally determined hardening curve.

Additionally, an assumption has been made, that the Young modulus is independent on applied strain rate (Figure 2).

Basing on previously illustrated laboratory results, the viscoplastic Chaboche's model has been proposed to capture the response of experimental samples on applied loading.

Model

The list of possible constitutive equations for the description of solid propellants is rather long, ([4-7]), and the choice of appropriately modeling of basic mechanical properties was based on observed experimental results and the easiness of determining the model parameters.

Although many publications deal with viscoplastic constitutive models [7], only a few focus on the procedures for determining the material constants. The Chaboche's model, developed from Perzyna viscoplastic equations [8], was originally proposed for metals, is relatively universal. In [9] and [10] the viscoplastic behavior of fabric textiles is modeled by using the Chaboche constitutive relation. It has been found, for example in [11], that the nonlinear behavior of polymers can also be modeled using this model. These considerations inspired us to choose the Chaboche viscoplastic constitutive law for the description of the mechanical properties of solid propellants.

Basing on formulations taken from [7], the Chaboche's equation for an uniaxial case can be presented in the following form

$$\sigma = k + \frac{2}{3}\frac{a}{c}\left[1 - \exp\left(-c\varepsilon_p\right)\right] + Q\left[1 - \exp\left(-b\varepsilon_p\right)\right] + K\dot{\varepsilon}_p{}^m, \qquad (3)$$

where:

σ – total stress,
ε_p – plastic strain,
$K|\dot{\varepsilon}_p|^m$ – viscous function,
k – initial yield limit (the yield point acquired in uniaxial experiment for strain independent strain rate),
Q – isotropic hardening parameter (responsible for cyclic hardening effects for Q>0 and softening effects when Q<0),
b – isotropic hardening exponent (the parameter responsible for convergence rate of the model to the stabilized cycle),
K – strain rate coefficient (the plastic strength function), m – strain rate or viscous exponent.
a,c – kinematic hardening function parameters.

Having in mind some postulations presented in [7] we can assume:

$$\varepsilon = \varepsilon_e + \varepsilon_p \tag{4}$$

$$\varepsilon_e = \frac{\sigma}{E} \tag{5}$$

where:
E – Young modulus,
ε_e – elastic strain.

Also:

$$\varepsilon_p = \varepsilon - \varepsilon_e\ , \tag{6}$$

and finally plastic strain rate:

$$\dot{\varepsilon}_p = \dot{\varepsilon} - \frac{1}{E}\dot{\sigma} \tag{7}$$

In this preliminary approach to the modeling process of viscoplastic response of homogeneous solid rocket fuels on external loading, authors omitted the influence of kinematic hardening. In that case, the final form of the Chaboche model can be written as

$$\sigma = k + Q\left[1 - \exp\left(-b\varepsilon_p\right)\right] + K\dot{\varepsilon}_p{}^m\ . \tag{8}$$

Parameters' identification using evolutionary algorithms

Viscoplastic phenomenological constitutive law proposed to model the behaviour of the material under consideration involving several parameters. The direct experimental determination of these constants is complicated and demands sophisticated and expensive conditions. However, the values of the model parameters may be obtained from the observed experimental results by solving numerically the corresponding inverse problem.

The parameters identification task can be formulated as an optimization problem. In fact, we dispose of a set of experimental data (represented by stress-strain curves) obtained for different strain rates. From the other side, the material behaviour may be simulated numerically (according to Chaboche law) for a given set of parameters values. Thus, the material constants can be found by comparing both approaches and by minimizing the differences between them. Thus, the sum of errors between experimental and calculated curves at some points of the investigated domain can be taken as objective function. The problem is to minimize this value by an appropriate choice of parameters' values. This way the curve fitting problem becomes the minimization problem. It can be formulated as follows:
determine N material parameters $c_1, c_2, ..., c_N$ of a given constitutive law
so as to minimize the sum F of squared differences between measured experimental data $\sigma^{\exp}$ and computed results σ^{num} at M given points of experimental domain $\varepsilon_i^{\exp}$

$$F(c_1,...,c_N) = \sum_{i=1}^{M} \left[\sigma_i^{\exp} - \sigma_i^{num}(c_1,...,c_N) \right]^2 \rightarrow \min \tag{9}$$

The solution of the parameters identification problem (8) will be carried out using evolutionary algorithm based on optimization procedure. It enables us to avoid difficulties encountered during the process of parameters identification by classical methods.

Evolutionary algorithms (EA) are stochastic search methods inspired by natural evolution, hereditary and survival of the fittest. They are general purpose techniques, adapted to find exact or approximate solution to unconstrained optimization tasks, especially efficient in the case of difficult problems [12, 13]. The EA processes at a time a fixed number (population) of candidate solutions, performing an efficient multi-directional exploration and exploitation of the design space. An encoded representation of the problem is applied (e.g. chromosome like structures). The evolution is simulated using a set of biologically inspired genetic operators (like selection, crossover, and mutation) and random parameters. The process continues for several iterations (generations) and better designs have a tendency to replace less efficient propositions. The final solution is determined by the design corresponding to the maximal fitness (a value that measures the quality of the represented solution).

The general algorithm of the method may be represented as the following scheme (more details can be found in [12, 13] or in the authors' paper [14]):

```
Generation of the initial population of potential solutions
Evaluation of the initial population (determination of fitness values)
When the termination condition is not satisfied do:
    Creation of new solutions by recombining individuals of the previous population
                        (selection of elements for mating, crossover and mutation)
    Evaluation of new solutions
    Selection of a new population
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The evolutionary algorithm, developed for this study, used the floating point, natural representation of design variables. The chromosome representation of a potential solution corresponded to the string of N searched material constants c_i (i=1,…,N). The material parameters of a population were processed in succeeding generations, tending to enhance the optimization criteria. The following fitness definition has been used in this study:

$$fitness(c_1,...,c_N) = \frac{s}{F(c_1,...,c_N)+1} \rightarrow \max . \tag{10}$$

Since the fitness value is usually maximized by the EA, the inverse of objective function F (9) has been applied. The unity term in the denominator is incorporated to avoid the singularity of the resulting expression, and s is a scaling coefficient.

In order to evaluate the population of potential solutions, the fitness of each individual is determined for a curve simulated numerically and compared with the experimental data. The searched parameters c_i (i=1,…,N) are generated within the range defined by the lower and the upper limits, and fixed by the user:

$$c_i^{\min} \leq c\text{i} \leq c_i^{\max} \qquad i = 1,...,N. \tag{11}$$

Numerical examples

The efficiency of EA based identification is studied for uniaxial tensile tests applied to homogeneous solid propellants specimens. The six material parameters

E, k, Q, b, K, m of the Chaboche model are determined numerically within the following variation limits: $1 \times 10^8 \leq Q \leq 5 \times 10^8$ [N/m^2], $10^4 \leq k \leq 10^6$ [N/m^2], $10^4 \leq Q \leq 10^6$ [N/m^2], $0 \leq b \leq 9 \text{x} 10^3$ [.], $10^3 \leq K \leq 10^7$ [.], $0.1 \leq m \leq 1.5$ [.]. The stress-strain curves have been simulated in the non-linear strain range. The objective function has been formulated by taking $M = 20$ "comparison" points regularly disposed over this domain.

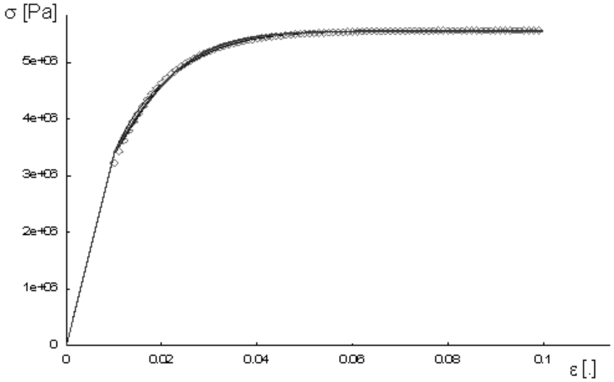

Figure 3. Results of 10 independent runs of EA identification for homogeneous solid propellant and strain rate $\dot{\varepsilon}_1 = 0.02$ [1/s].

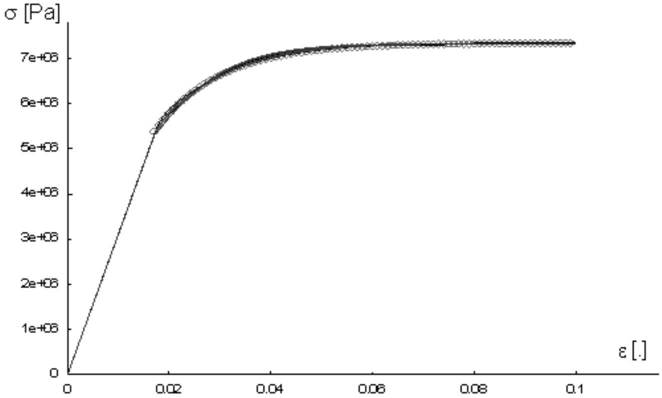

Figure 4. Results of 10 independent runs of EA identification for homogeneous solid propellant and strain rate $\dot{\varepsilon}_1 = 0.002$ [1/s].

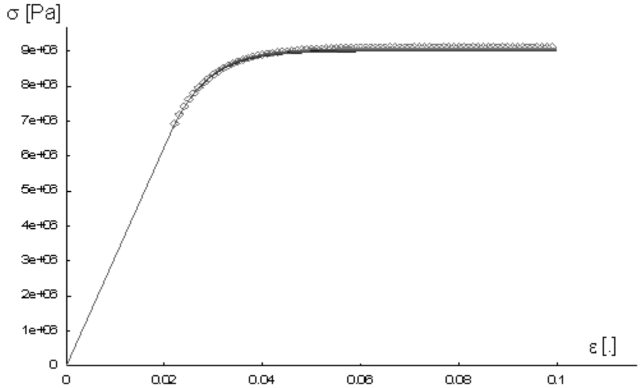

Figure 5. Results of 10 independent runs of EA identification for homogeneous solid propellant and strain rate $\dot{\varepsilon}_1 = 0.0002$ [1/s].

The evolutionary algorithm applied the population of 60 individuals, the "single" arithmetical crossover operator (with 60% probability), the non-uniform mutation (with 15% probability). 200 generations have been investigated and the selection procedure employed the tournament ranking using random pairs. Moreover, the elitist approach replaced 10 worst individuals in the new generation by 10 best individuals found in the previous generation. In order to determine a solution, the evolutionary procedures apply random numbers. In consequence, similar (but not identical) results are produced at every run of the algorithm. Thus, the robustness of the EA identification is investigated by running the program independently 20 times and by studying the average values.

In Figures 3, 4, 5, the average results obtained in 10 independent runs of the EA identification program are presented for strain rates $\dot{\varepsilon}_1 = 0.02$ [1/s], $\dot{\varepsilon}_2 = 0.002$ [1/s], and $\dot{\varepsilon}_3 = 0.0002$ [1/s], respectively. Estimated parameters values for considered strain rates are given in Table 1.

Table 1. Values of model parameters for various strain rates

Strain rate [1/s]	E [Pa]	k [Pa]	Q [Pa]	b [-]	K [-]	m [-]
0.02	$3.4 \cdot 10^8$	$4.4 \cdot 10^5$	$1.6 \cdot 10^6$	130	$9.6 \cdot 10^6$	0.26
0.002	$3.7 \cdot 10^8$	$3.3 \cdot 10^6$	$2.1 \cdot 10^6$	100	$9.8 \cdot 10^6$	0.26
0.0002	$3.2 \cdot 10^8$	$3.2 \cdot 10^4$	$5.7 \cdot 10^6$	$9.9 \cdot 10^3$	$4.2 \cdot 10^8$	0.57

One can see that the applied stochastic method gives very good solutions. Different values of material parameters describe subsequent hardening curves.

This way, the proposed constitutive model is able to describe the behavior of considered materials.

Several independent runs of the EA identification program have been carried out for each example, leading to very similar results.

Conclusions

The results of uniaxial tensile experiments, conducted on samples made of homogeneous solid propellant, are correctly represented by the curves corresponding to numerical modeling. The EA based methodology, presented in the paper for parameters' identification of the Chaboche's law, is quick and effective. Additional improvement of the convergence can be achieved by reducing the explored range of parameters' variations. Moreover, the experimental determination of basic strength characteristics (like E and k) could simplify considerably the simulation problem.

The presented work has to be interpreted as an initial investigation of the modeling of solid propellants nonlinear properties. The viscoplastic constitutive model applied in this study was suitable for the phenomenological description of the physical behavior of the analyzed material. Although it is impossible at this stage to estimate the global impact of the strain rate on models parameters, the obtained results encourage further works on numerical simulation and modeling of solid propellants.

The applied methodology can be easily adapted to other experiments and different constitutive models or various kinds of investigated problems (temperature and strain rate influence, cycling loading, etc.).

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