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Quasi-static Tension-compression Nonlinear Constitutive Model of TATB-based PBX and its Application

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Abstract: The stress-strain curves of polymer bonded explosives (PBXs) are generally nonlinear and poorly unsymmetric. The construction of constitutive model is a difficult problem in the research of mechanical properties of explosives. In this paper, taking PBX-901 as the research object, the uniaxial tension and compression experiments at different temperatures were carried out firstly. Then, a four-parameter and a two-parameter constitutive model were respectively established and the relative undetermined parameters were determined based on the Boltzmann function according to S-shaped stress-strain curves obtained. The parameters of two-parameter constitutive model can be determined only using analytical solution including the compression strength and initial segment elastic modulus, and its description error is less than 5%, while the parameters of the four-parameter model though parameter fitting. Finally the second development module of ANSYS software was adopted to realize the numerical application of the two-parameter constitutive model for the Brazilian disk tests. Through comparison with the experimental results, the relative error of numerical results only is about 5.11%. The description precision of the nonlinear two-parameter constitutive model established in the text is satisfactory and it meets the needs of engineering.

Key words: polymer bonded explosive (PBX); nonlinear constitutive model; Boltzmann function; S-shaped stress-strain curve; Brazilian disk test

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1 Introduction

The constitutive model for materials is the basis of numerical simulation to explain the macro phenomena and predict the mechanical responses of structures, and always can be expressed through the mathematical expression of the material stress-strain relationship. Up to now, constitutive modeling is still a hotspot in mechanical research of solid materials, including the polymer bonded explosives (PBXs) as for their evident nonlinearity and asymmetry of the tensile and compression curves[1-3]. The tension-compression stress-strain curves of PBXs are always S-shaped curves. In previous studies[4-5], the tension-compression constitutive models of PBXs were processed independently. Actually, accurately describing the tension-compression nonlinear constitutive behavior of PBX is still a major challenge in mechanical research of explosives. On one hand, the tension-compression nonlinear constitutive model of PBX has to exhibit satisfactory mathematical description accuracy. On the other hand, model parameters should have explicit physical significance and their initial values should be determined easily.

Research on the PBX constitutive model can be dated back to 1984. Browning investigated the PBX constitutive model in 1984[6] and optimized this model in 1989[7]. However, this constitutive model is only a one-dimensional model. The statistical microcrack model (SCRAM) is a well-known model used to analyze the constitutive behavior of solid brittle materials

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in recent years[8-9]. This model has been extensively used in rocks and concrete. As a constitutive model based on microcrack damages and statistical theory, SCRAM could reflect the physical process of material internal response under stress to a certain extent, which is conducive to determine the micro-deformation mechanism of inner materials. The ViscoSCRAM model[10-12] is the most well-known PBX constitutive model and is still being used widely at present. In this model, not only the advantages of the SCRAM model are inherited, but also the viscoelasticity of PBX material is considered. However, the ViscoSCRAM model is disadvantageous and inconvenient to apply as for that too much numerous parameters need to be determined. Besides, this model could also not provide a satisfactory practical application effect, and its practicability still needs to be improved. Though many other works on constitutive behavior of explosives has been reported[13-15] recently, but as reported by Shunk in 2014, "even with all of the exploratory works, the constitutive models for PBXs are still lacking."[16] In this study, a type of quasi-static tension-compression nonlinear constitutive model is discussed based on our early work[17], and its parameters are determined according to test data. Numerical implementation of this model is accomplished in the finite element software, then the accuracy of this model is evaluated by the comparison between Brazilian disk tests and their simulation results.

2 Experiment

2.1 Materials and Instruments

PBX-901, a typical [1,3,5-triamino-2,4,6-trinitrobenzene] (TATB)-based PBX composed of TATB explosive crystal (>94% mass ratio) and fluorous rubber (<6% mass ratio) in China, was used as the research object in this study. Uniaxial tension and compression tests were performed on a Instron-5582 material testing machine. Tensile dumbbell samples (Φ15 mm × 65 mm) and compressed cylinder samples (Φ20 mm × 20 mm) met the associated requirements of the GJB772A-1997 standard of China.

2.2 Test Method and Data Processing

The uniaxial tension tests and uniaxial compression tests were conducted at 20, 25, 30, 35, 40, 45 ℃ and 50 ℃ respectively. Three samples were tested in parallel at each temperature. The test method met the GJB772A-1997 standard of China.

Acquired test data were processed in two steps. First, test data including stress and strain (positive for tension and negative for compression) were recorded. The curve from zero stress to the maximum tensile/compressive stress (numerical value regardless of the signs) was viewed as the stress-strain curve of the tension/compression segment. Then, the tension and compression stress-strain curves were drawn in the same coordinate system. Figure 1 shows the whole stress-strain curves of PBX-901 considering tension and compression at 20 ℃. According to the proposed stress-strain curves, the arithmetic mean values of tensile strength (σ_t), compression strength (σ_c), and elastic modulus close to zero strain (E_0) of the three PBX-901 samples under the same experimental environment were calculated. Curves at other temperatures have a similar shape with those shown in Fig. 1, but different numerical values.

The results at different temperatures are listed in Table 1. From the Table 1, we can get that all the

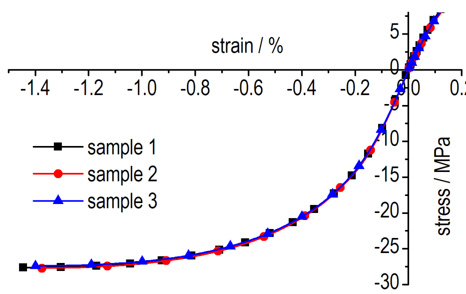


Fig. 1 Tension-compression stress-strain curves of PBX-901 at 20 ℃

Table 1 Mechanical parameters of PBX-901 at different temperatures

temperature /℃	tensile trength /MPa	compression strength /MPa	E_0 /GPa
20	8.56	-27.58	7.37
25	8.26	-25.31	7.20
30	7.69	-24.46	6.80
35	7.48	-22.35	6.4
40	7.11	-20.52	6.06
45	6.61	-19.86	5.95
50	6.38	-17.58	4.88

mechanical constants (tensile strength, compression strength and Young's modulus) decrease with increasing the test temperature.

3 Characteristics of the Stress-strain Curve and Constitutive Model

3.1 Characteristics of the Stress-strain Curve

Figure 1 shows in complete sigmoid shape stress-strain curves of PBX-901 which can be divided into three stages mathematically, namely, low stress, middle stress and high stress stages. In the low stress stage, the stress-strain curve is nearly a straight line and the tangent modulus which is defined as stress variation / strain variation is approximately a constant higher than zero. In the middle stress stage, the tangent modulus decreases gradually, and the maximum bearable stress of the sample occurs when decreasing to zero. In the high stress stage, stress decreases gradually while strain increases continuously , that is, the tangent modulus further decreases into negative until the final sudden failure. Compression process has all the three stages while tensile process only includes low stress stage.

3.2 Deduction of the Constitutive Model

A S-shaped function is need to describe the stress-strain curves. Boltzmann sigmoid, Gaussian cumulative, and Lorentz cumulative are three typical S-shaped curve functions often used to describe the transition behavior of a physical parameter. These functions have been extensively applied in medicine, biology, agriculture, physics, and chemistry[18-19]. Their mathematical expressions are shown in Eqs. (1), (2) and (3) respectively. In these equations, x is an independent variable and y is a dependent variable. The parameters of the three equations have different physical significance. Four coefficients, namely, Y_1, Y_2, x_0, and dx, represent the theoretical lower limit, theoretical upper limit, independent variable midpoint, and slope correlation coefficient of function y, respectively. Slope value at x_0 is $(Y_2-Y_1)/4dx$. The three functions used different mathematical forms to describe the same S-shape curve (Fig. 2). In this study, the Boltzmann function with simpler form and wider application was used to deduce the constitutive model.

$$y(x) = \frac{Y_1 - Y_2}{1 + e^{(x - x_0)/dx}} + Y_2 \tag{1}$$

$$y(x) = \frac{(Y_2 - Y_1).\arctan\left(\left(\left(x - x_0\right)/dx\right) + (\pi/2)\right)}{\pi} + Y_1 \tag{2}$$

$$y(x) = \frac{Y_2 - Y_1}{2}\left(1 + \frac{2}{\sqrt{\pi}}\int_0^{\frac{x - x_0}{\sqrt{2}dx}} e^{-t^2}\, dt\right) + Y_1 \tag{3}$$

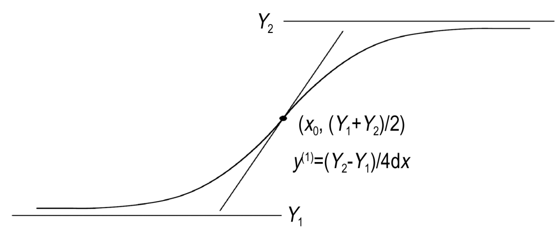


Fig. 2 Typical S-shaped curve and physical significance of parameters

A four-parameter Boltzmann constitutive model (Eq.(4)) could be generally derived from Eq.(1) as shown in Eq.(4), σ and ε are the stress and strain, respectively (positive for tension and negative for compression); σ_{tll}, σ_{tul}, β, and α are the theoretical lower stress limit, theoretical upper stress limit, correction factor at zero stress-strain point, and correlation coefficient of the modulus, respectively; and β and α are dimensionless numbers. Undetermined coefficients in this model have explicit physical significance.

$$\sigma = \frac{\sigma_{tll} - \sigma_{tul}}{1 + e^{\alpha\varepsilon + \beta}} + \sigma_{tul} \tag{4}$$

According to the curve characteristics shown in Fig. 2 and the physical significance of parameters, the initial values of the undetermined coefficients in Eq.(4) could be derived easily through the following methods:

(1) σ_{tll} is selected as the compression strength σ_c, and the initial value of σ_{tul} is higher than the tension strength σ_t, which is a virtual value that is beyond reach. σ_t can be taken as $-\sigma_c$.

(2) The zero point correction coefficient β is used to ensure that zero strain corresponds to zero

stress. Based on Eq.(4), the initial value (β_0) can be expressed as follows:

$$\beta_0 = \ln\left(-\frac{\sigma_{tll}}{\sigma_{tul}}\right) \tag{5}$$

(3) According to the definition of the modulus, the expression of the elastic modulus (Eq.(6)) could be derived from Eq.(4). Based on Eq.(6), the initial value of the modulus correlation coefficient of zero strain (α_0) can be derived (Eq.(7)) as follows:

$$E = \frac{d\sigma}{d\varepsilon} = -\frac{\alpha e^{\alpha\varepsilon+\beta}\left(\sigma_{tll} - \sigma_{tul}\right)}{\left(1 + e^{\alpha\varepsilon+\beta}\right)^2} \tag{6}$$

$$\alpha_0 = \frac{E_0\left(1 + e^{\beta}\right)^2}{e^{\beta}\left(\sigma_{tul} - \sigma_{tll}\right)} \tag{7}$$

where E_0 is the elastic modulus value close to the zero point.

In particular, if the tension and compression stress-strain curves of the material are symmetric, that is, σ_{tul} is equal to σ_{tll} in numerical value and has opposite signs ($\sigma_{tll} = -\sigma_{tul} = \sigma_c$ and $\beta = 0$), then the mathematical expression can be simplified into the two-parameter Boltzmann constitutive model expressed in Eq.(8). σ_c can be tested directly and the undetermined coefficient α can be fitted or calculated by Eq.(9).

$$\sigma = \frac{2\sigma_c}{1 + e^{\alpha\varepsilon}} - \sigma_c \tag{8}$$

$$\alpha_0 = -\frac{2E_0}{\sigma_c} \tag{9}$$

3.3 Establishment of the Constitutive Model

As shown in Figs. 3 and 4, test data of PBX-901 at 20 ℃ and fitting results with the four-parameter Boltzmann constitutive model (Eq.(10)) and the two-parameter model (Eq.(11)) were compared. The mean-adjusted R^2 values between test data and fitting data in Figs. 3 and 4 are 0.99852 and 0.99712, respectively. This result shows both the fitting curves with both models are highly consistent with the test data, and the description accuracy with four-parameter model (Fig. 3) is slightly higher.

$$\sigma = -\frac{69.38}{1 + e^{4.669\varepsilon - 0.441}} + 42.26 \tag{10}$$

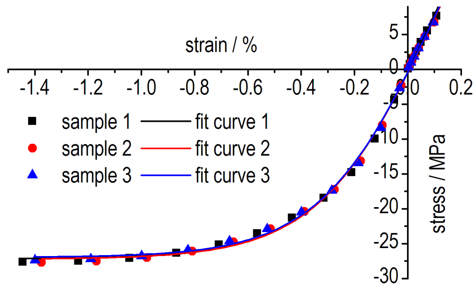


Fig. 3 Comparison of the tests and fitting results of the four-parameter Boltzmann constitutive model of PBX-901 at 20 ℃

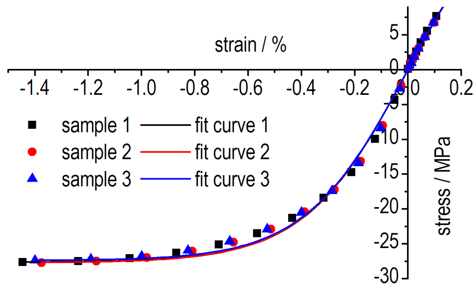


Fig. 4 Comparison of the tests and fitting results of the two-parameter Boltzmann constitutive model of PBX-901 at 20 ℃

$$\sigma = -\frac{55.16}{1 + e^{5.158\varepsilon}} + 27.58 \tag{11}$$

According to the analysis presented in Section 3.2, σ_c in the two-parameter Boltzmann constitutive model (Eq.(8)) can be obtained directly from the test (Table 1). According to Eq.(9), α_0 is 534.45 at 20 ℃ using true strain expression, and it is 5.345 when expressed by percentage strain. This result is approximately 3.625% higher than the fitting one (5.518). Actually, the parameters of the two-parameter Boltzmann constitutive model were not fitted, but the analytic results ($\sigma_c = -27.58$ MPa and $\alpha_0 = 5.345$) were adopted, which can also provide satisfactory description accuracy (Fig. 5). When calculating the analytical results of the parameters, σ_c and E_0 are needed, whereas the tensile curve is unnecessary. In other words, the two-parameter Boltzmann constitutive model of PBX-901 considering tension and compression can be established even if no tension test and data fitting have been conducted.

The simulation results of PBX-901 (parameter used fitting values and analytic values) were compared with the test ones (Figs. 6 and 7) at 50 ℃ to

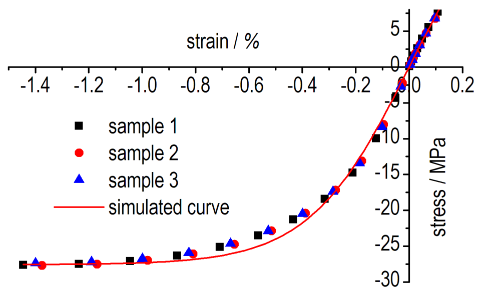


Fig. 5 Comparison of the the tests and simulated curve by the two-parameter Boltzmann constitutive model with parameter values based on analytic results at 20 ℃

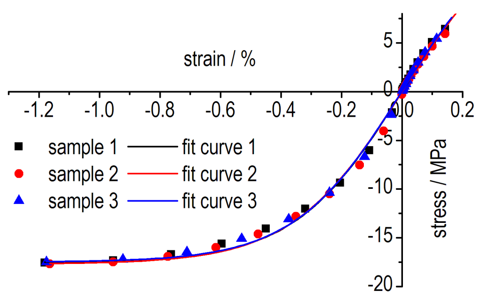


Fig. 6 Comparison of the tests and fitting results of the two-parameter Boltzmann constitutive model of PBX-901 at 50 ℃

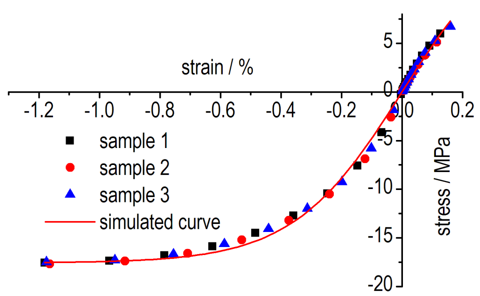


Fig. 7 Comparison of the tests and simulated curve by the two-parameter Boltzmann constitutive model with parameter values based on analytic results at 50 ℃

verify the applicability of the two-parameter constitutive model at different temperatures. The fitting values of σ_c and α were −17.58 MPa and 5.566, respectively, whereas the analytic values were −17.58 MPa and 5.552, respectively. The difference of α was only approximately 0.252%.

According to the previously presented analysis, the two-parameter Boltzmann constitutive model could accurately describe the compression constitutive behavior of PBX-901. However, this model can only describe constitutive behavior when stress and strain increase (numerical value) simultaneously, but could not describe the phenomenon when stress decreases and strain increases after the maximum compression load. The parameter values of the two-parameter Boltzmann constitutive model within 20−50 ℃ are shown in Table 2.

Table 2 Parameters of the two-parameter Boltzmann constitutive model at different temperatures

temperature /℃	compression strength /MPa	modulus correlation coefficient
20	−27.58	5.158
25	−25.31	5.171
30	−24.46	5.183
35	−22.35	5.195
40	−20.52	5.226
45	−19.86	5.361
50	−17.58	5.566

4 Numerical Simulation and Application of the Model

4.1 Secondary Development of the Two-parameter Boltzmann Constitutive Model

The secondary development of the two-parameter Boltzmann constitutive model is based on user-programmable features (UPFs) and usermat subroutine of the ANSYS software. Through UPFs, user-defined material, element and failure criterion (for composites) can be realized through programming corresponding subroutine using FORTRAN language. There are three steps to finish a material subroutine. First, the equivalent strain from stress is calculated according to the constitutive model (Eq.(8)). Secondly, the stiffness and Jacobian matrices are calculated according to the equivalent strain. Finally, the secant modulus is used instead of the elasticity modulus in the stiffness and Jacobian matrices to calculate and update current stress. These steps will be repeated in numerical simulation until the end of computation. Specially, the tangent slope is calculated to replace the secant modulus as for that it's difficult to calculate when strain is close to zero. This program could be applied in the ANSYS software after being compiled.

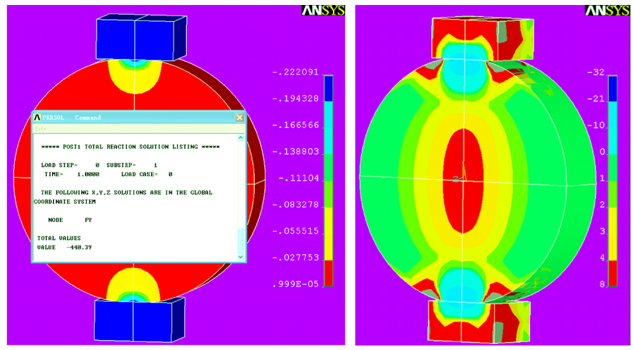
4.2 Numerical Simulation of the Brazilian Disk Test

To verify the description accuracy of the two-parameter Boltzmann constitutive model in practical engineering, the Brazilian disk test was performed and simulated. The Brazilian disk test is extensively used in investigating the mechanical performances of explosive materials. The test in this study was conducted at 20 ℃ by using three Φ25 mm × 10 mm compressed samples. Sample size and test results are presented in Table 3. The test results show that the average size is Φ24.903 mm × 9.997 mm. Moreover, the average values of critical load and load displacement are almost 1856.441 N and 0.444 mm respectively.

Table 3 Sample size and Brazilian disk test results

sample number	diameter /mm	thickness /mm	critical load /N	load displacement /mm
1	24.90	10.00	1814.641	0.441
2	24.91	9.97	1855.274	0.442
3	24.90	10.02	1899.408	0.449
average	24.903	9.997	1856.441	0.444

According to the symmetric relationship between stress and boundary conditions in the Brazilian disk test, a simulating model with 1/2 thickness and 1/4 perimeter was established. The mean sample size and model parameters at 20 ℃ were used as the input. The SOLID185 element, which is a 8-node finite element, was applied during modeling. During numerical simulation, the tested loading displacement was used as input. Thus, the description accuracy of the two-parameter Boltzmann constitutive model in practical engineering was reflected by the difference between calculated node counterforce of the pressing plate and the tested critical load. According to the symmetric relationship of the model, the plate displacement input in numerical simulation was 0.222 mm. The displacement field, node counterforce, and the first major principal stress output at this moment are shown in Fig. 8. The total node counterforce of the pressing plate is four times that of the model output (440.39 N) and reaches 1761.56 N while the test critical load is 1856.441 N. The relative error is only approximately 5.11% which reflects that the established two-parameter Boltzmann constitutive model has satisfactory description accuracy.



a. displacement distribution **b.** the first major principal stress distribution

Fig. 8 The simulation outputs according to the Brazilian disk test

5 Conclusions

A type of quasi-static tension-compression nonlinear constitutive model was deduced by using Boltzmann function in the present work, whose undetermined parameters show explicit physical significance and can be easily determined. Meanwhile, the two-parameter Boltzmann constitutive model was further deduced based on the symmetry of curves, and there are two ways to determine the initial parameter values. One is by fitting with test result and the other just using the compression strength and the initial modulus.

According to the test data, the four-parameter and two-parameter Boltzmann constitutive models of PBX-901 were established under different temperatures. Through analysis, both models showed satisfactory description accuracy. Besides, the two-parameter constitutive model shows a small difference between analytic and fitting parameter values, which indicates that just two physical constants, compression strength and modulus value, from conventional compression test are adequate to establish the high-accuracy tension-compression nonlinear constitutive model, and the tension test is no longer necessary. What's more, based on the UPFs platform of ANSYS software, a material subroutine of the two-parameter model was developed and the numerical simulation of the Brazilian disk test was performed, which used loading displacement as the input and critical load as the output. The simulation result shows only 5.11% relative error compared with the test results. This small error confirmed the high description accuracy of the two-parameter model in practical applications.

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TATB基PBX的准静态拉压非线性本构模型及其应用

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摘　要: 高聚物粘结炸药(PBX)的应力应变曲线普遍存在非线性显著和对称性较差的特点,本构模型构建困难是炸药材料力学性能研究中的一个难题。以PBX-901为研究对象,开展了不同温度下的单轴拉伸和单轴压缩试验,根据获得的S型应力应变曲线,基于Boltzmann函数分别推导建立了一种四参数本构模型和一种双参数本构模型。结果表明:较之于四参数本构模型,双参数本构模型的参数确定不需要参数拟合,仅采用压缩强度和初始段弹性模量解析求解的方式获取即可,描述精度误差低于5%。最后采用ANSYS软件的二次开发模块,实现了双参数本构模型在巴西圆盘试验中的数值模拟应用,试验结果和数值模拟结果的对比分析显示二者的相对误差仅5.11%,表明所建立的双参数本构模型的描述精度满足工程需要。

关键词: 高聚物粘结炸药(PBX);非线性本构模型;Boltzmann函数;S型应力应变曲线;巴西圆盘试验

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