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Research paper

A Pressure-Dependent Plasticity Model for Polymer Bonded Explosives under Confined Conditions

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Abstract: The safety of explosives is closely related to the stress state of the explosives. Under some stress stimulation, explosives may detonate abnormally. It is of great significance to accurately describe the mechanical response of explosives for the safety evaluation of explosives. The mechanical properties of polymer bonded explosives (PBXs) strongly depend on pressure. In this study, the mechanical behaviour of PBXs under confined conditions was investigated. It was found that the stress-plastic strain response of a PBX under high confining pressures is a combination of the non-linear and linear hardening portions. However, the linear hardening portion has often been neglected in characterizing the mechanical behaviour of a PBX under such pressures. The Karagozian and Case (K&C) model was applied to characterize the mechanical behaviour of PBXs. The numerical results demonstrated that when the confining pressure was high, the K&C model could not adequately match the experimental data due to the limitation of the damage model. Therefore, a new damage model was developed by means of considering intragranular damage and transgranular damage. This modification made it possible to introduce a linear hardening process into the original K&C model. The method proposed to describe the stress-strain results under high confining pressures was to consider the stress-plastic strain curve, including the nonlinear and linear hardening portions. The damage evolution of the original K&C model and a linear hardening model were applied for the nonlinear and linear hardening portions respectively.

The influence of the linear hardening model on the damage evolution of the original K&C model was included when describing the nonlinear hardening portion. A comparison between simulation and experiment showed that the modified K&C model could well describe the mechanical response of PBXs under different confining pressures.

Keywords: polymer bonded explosives, constitutive model, damage model, confining pressure, mechanical response

1 Introduction

Polymer bonded explosives (PBXs) are highly particle-filled composite materials, consisting of ‘hard’ crystal grains and ‘soft’ polymeric composites [1]. PBXs have a complex microstructure, and considerable microcracks are produced during the manufacturing process. Processing results in complex deformation mechanisms, such as grain-matrix interface debonding and grain microcracking, which make it difficult to describe PBXs’ mechanical behaviour. In the triaxial stress states, the mechanical behaviour of PBXs becomes more elusive. During axial compression under a 20 MPa confining pressure, an abundance of closed crack sliding and grain buckling was observed. When the confining pressure was increased up to 200 MPa, grain microcracks were completely closed. The grain behaves plastically, which is different from the case with no confining pressure [2]. Under some extreme conditions, such as impact, the deformation and damage in PBXs occurring under confining pressures may lead to ignition and other dangerous events. Therefore, an understanding and modelling of the mechanical responses under confinement is of considerable interest for the safety assessment of PBXs [3-5].

The constitutive models describing the mechanical behaviour of PBXs are generally classified into two categories. One category is developed on the basis of the deformation mechanisms of the materials. The typical mechanism-based model is the Viscous Statistical Crack Mechanism model (Visco-SCRAM) proposed by Bennett *et al.* [6]. The Visco-SCRAM model combines a viscoelastic component with a continuum crack evolution component. Each component in the model has a physical meaning. The model can describe the viscoelastic response and the crack evolution of PBXs [7]. However, the deformation mechanisms of PBXs are very complex, and some are not even understood clearly, so there exist some limitations with such models in the description of some deformations, especially under complex stress states. Rangaswamy *et al.* [8] checked the validity of the Visco-SCRAM model under

different loading conditions and pointed out that, since the evolution of the crack did not take into account the effect of hydrostatic pressure and was only affected by the deviatoric stress, the model was only suitable for simulating the failure of the explosives in the case of uniaxial loading in nature, with little influence of pressure. The other category is a macroscopical mechanical response model. The High Explosive Response to MEchanical Stimulus model (HERMES) proposed by Reaugh [9, 10] and the viscoplastic model by Gratton *et al.* [11] are in this category. In these models, the mechanical behaviour of PBXs is primarily characterized by the strength surfaces and damage evolution, which depend on plastic strain, pressure *etc.* These models describe the macroscopic stress-strain responses only and do not consider the deformation mechanisms. Obviously, it is feasible and easy to describe the mechanical behaviour of PBXs for these models, especially under complex stress states. Despite the above advantage, unfortunately, these models do not give satisfactory results when the confining pressure is high. There seems to be no effective description method due to the complexity of the microstructures. Moreover, it is difficult to establish the direct relationship between the meso-deformation process and the macro-mechanical response. Modelling of the mechanical response of PBXs using the second category of model is thus often of practical interest, especially when the hardening behaviour is sensitive to the confinement.

The Karagozian and Case (K&C) model proposed by Malvar *et al.* [12], the Riedel-Hiermaier-Thoma (RHT) model by Riedel, Thoma and Hiermaier *et al.* [13], and the Holmquist-Johnson-Cook (HJC) model by Holmquist, Johnson and Cook *et al.* [14, 15], *etc.* have been developed as typical phenomenological models. These models belong to the above second category of constitutive model and are widely used in commercial software. However, these models cannot capture the linear hardening characteristics of PBXs under a high confining pressure greater than the brittle-to-ductile transition point. The experimental results [2, 3] showed that under high confining pressures, the linear hardening behaviour was presented in the stress-plastic strain curve of the PBXs, and the hardening slope varied with the confining pressure. These models describe the phenomenon by means of the damage evolution models. The simulation results could not be perfectly matched with experimental results. Moreover, in the case of high confining pressures, the maximum stress value cannot be determined in the stress-plastic strain curve due to the appearance of the linear hardening behaviour. Furthermore, it is hard to determine the parameters of the maximum strength surface in these models. Wiegand *et al.* [16, 17] suggested applying the flow stress as the maximum value. The flow stress was taken at the intersection

of the linear hardening portion and the initial portion of the stress-strain curve. However, Vial *et al.* [18] believed that the stress peak of the stress-strain curve should exist, but it might not be obtained due to the capacity limitation of the apparatus. There is still no unified understanding of the maximum stress value under high confining pressures. In order to characterize the mechanical behaviour of a PBX well, it is necessary to solve this problem.

In the present study, the K&C model was selected as the basic framework for the constitutive modelling due to its good extendibility, and was modified for describing the mechanical behaviour of PBXs under a wide range of confining pressures. A new damage model, considering both intragranular damage and transgranular damage, was developed, making it possible to introduce a linear hardening process into the K&C model. Determination of the pressure dependent parameters in the modified model is discussed. The simulation of the mechanical response of PBXs under various confining pressures was conducted using the model and was compared with experimental data for the validation of the modified K&C model.

2 The K&C Model

The K&C model was developed based on the Pseudo-tensor model [12]. It includes the implementation of tensile and compressive asymmetry, strain rate effect, pressure dependent behavior, *etc.* The model is used to describe the mechanical response behaviour of the material through three strength surfaces combined with the damage parameter or the interpolation function. The model [19] has been successful in describing the mechanical behaviour of concrete materials, which is similar to PBXs.

2.1 Strength surfaces

The method to determine the current yield strength of materials by means of special strength surfaces (or failure surfaces) is widely used. The stress states at the three special points of the stress-strain curve (see Figure 1) are applied as the special strength surfaces. The stress-strain curve could be obtained by means of nonlinear or linear interpolation among the three points.

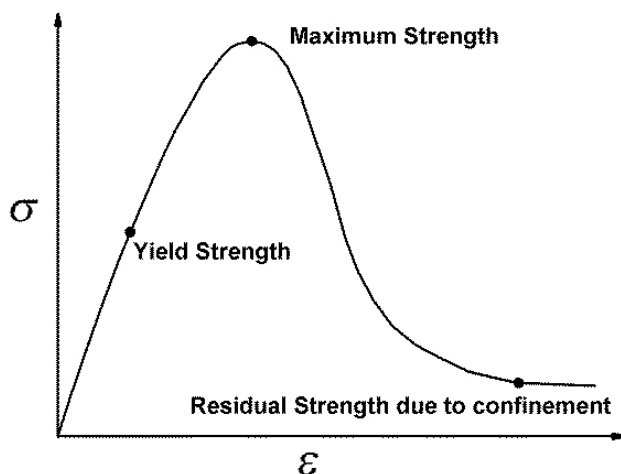


Figure 1. The stress-strain curve of a material

In the stress space, the three feature points represent three strength surfaces. The strength surfaces in the model are described by the combination of tension or compression meridian and deviatoric plane (a description method similar to a cylindrical coordinate system in the stress space). When the hydrostatic pressure is beyond $f_c/3$, the compressive meridian (see Figure 2) is input as the basis. f_c is the uniaxial compression strength of the material. The expressions of the three compression meridians (corresponding to the three strength surfaces) are:

$$\Delta\sigma_m = a_0 + p_m/(a_1 + a_2 p_m) \quad (\text{Maximum strength}) \quad (1)$$

$$\Delta\sigma_r = p_r/(a_{1f} + a_{2f} p_r) \quad (\text{Residual strength}) \quad (2)$$

$$\Delta\sigma_y = a_{0y} + p_y/(a_{1y} + a_{2y} p_y) \quad (\text{Yield strength}) \quad (3)$$

where a_0 , a_1 , a_2 , a_{1f} , a_{2f} , a_{0y} , a_{1y} and a_{2y} are all input parameters, and p_m , p_r and p_y are the hydrostatic pressures corresponding to maximum strength, residual strength, and yield strength, respectively. $\Delta\sigma$ is the principal stress difference, and it is often used to describe the stress response with the confining pressure. The hydrostatic pressures are linked by the interpolation path (the broken lines in Figure 2). Note that the residual strength should not be beyond the maximum strength. Here the hydrocode convention is used where positive pressure and negative stress deviators are compressive.

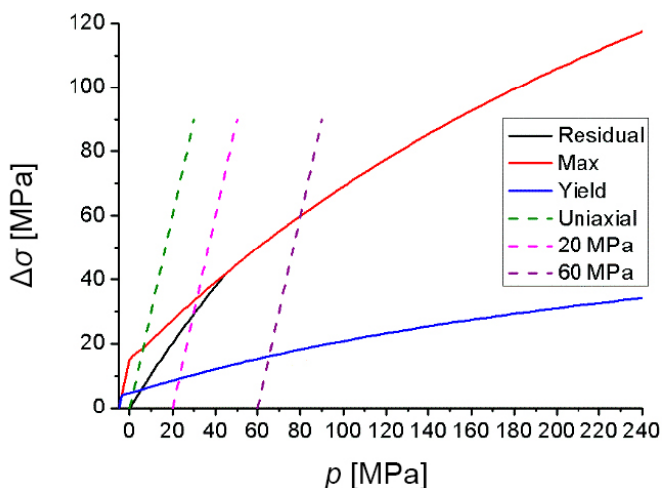


Figure 2. Compression meridian and the interpolation path

When the hydrostatic pressure is below $f_c/3$, the tension meridian is input as the basis, because many tests were associated with the tension meridian (uniaxial tension, biaxial compression, *etc.*) in this region. The expression is:

$$\Delta\sigma = 3/2(p_m + f_t) \quad (\text{Maximum strength}) \quad (4)$$

where f_t is the uniaxial tension strength of the material.

The deviatoric plane in the K&C model is described by William-Warnke's formula [20]:

$$r' = \frac{2(1-\Psi^2) \cos\theta + (2\Psi-1)\sqrt{4(1-\Psi^2) \cos^2\theta + 5\Psi^2 - 4\Psi}}{4(1-\Psi^2) \cos^2\theta + (2\Psi-1)^2} \quad (5)$$

$$r' = r/r_c,$$

$$\Psi = r_t/r_c,$$

where r_c is the distance from the hydrostatic pressure axis to the strength surface at the compression meridian, r_t is the distance from the hydrostatic pressure axis to the strength surface at the tensile meridian, r ($r_t < r < r_c$) is the distance at any intermediate position, and θ is the Lode angle, and its value can be calculated by means of the following equation:

$$\cos\theta = (\sqrt{3}s_1)/(2\sqrt{J_2}) \quad \text{or} \quad \cos 3\theta = (3\sqrt{3}J_3)/(2J_2^{3/2}) \quad (6)$$

$$J_2 = 1/2(s_1^2 + s_2^2 + s_3^2)$$

$$J_3 = s_1s_2s_3.$$

where s_1 , s_2 and s_3 are the principal stress deviators. A schematic diagram of the deviatoric plane in the K&C model is shown in Figure 3. The deviatoric plane is perpendicular to the hydrostatic pressure axis, and describes the ratio of the strength surface to the compression meridian under a specific hydrostatic pressure. In this way, the strength surface of the material can be completely described by the compression meridian and the deviatoric plane.

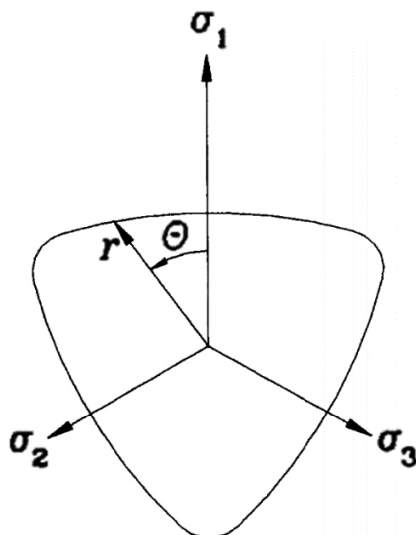


Figure 3. The schematic diagram of the deviatoric plane in the K&C model [12]

2.2 Interpolation function (damage evolution curve)

The interpolation function $\eta(\lambda)$ in the K&C model is used to determine the current yield strength of the material. It is a function of the damage parameter λ . The damage evolution in the model is decomposed into two parts, the nonlinear hardening response (by interpolating between the yield and maximum strength) and the nonlinear softening response (by interpolating between the maximum and residual strength). The two different responses are determined by means of the critical value of the damage parameter λ_1 corresponding to the maximum $\eta(\lambda)$. The expression of the current compression meridian of the material is:

$$\begin{cases} \Delta\sigma = \eta(\lambda)(\Delta\sigma_m - \Delta\sigma_y) + \Delta\sigma_y & \lambda \leq \lambda_1 \\ \Delta\sigma = \eta(\lambda)(\Delta\sigma_m - \Delta\sigma_r) + \Delta\sigma_r & \lambda > \lambda_1 \end{cases} \quad (7)$$

The damage parameter λ is:

$$\lambda = \int_0^{\varepsilon_p} d\varepsilon_p / (R_{DIF}(1 + p/(R_{DIF}f_t))^{b_1}) \quad (8)$$

where R_{DIF} is the dynamic increase factor (input values dependent on strain rate, 1 for quasi-static conditions), b_1 is a parameter that needs to be determined. The damage parameter λ is mainly based on the plastic strain, taking into account the effect of the hydrostatic pressure p . It can describe the effect of different hydrostatic pressures on the stress-strain responses of the material.

The interpolation function $\eta(\lambda)$ with respect to the damage parameter λ was directly given. The increment of the damage parameter λ could be given in an explicit form, which avoids the non-convergence problem in the implicit form calculation [12]. Equations 1-8 are taken from [12], which are the equations in the K&C model used in the present paper. The calculation of deviatoric stress and plastic strain increment in the model is based on the Prandtl-Reuss plastic flow assumption following the “radial return” algorithm [21].

2.3 Stress-strain response analysis

There are many kinds of PBXs. For different PBXs, the strength, modulus and so on would be very different, but the shape of the stress-strain curve is basically the same. Under a low confining pressure, the stress-strain curve would soften. However, the softening would disappear when the confining pressure was high. In this section, the stress-strain response of an octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (octogen, HMX) based PBX was analyzed. Its mechanical response is similar to the behaviour of PBX9501. The experimental data were taken from work performed by CEA researchers [2, 3, 11, 18]. The analysis results were mainly applied to understand the stress-strain response characteristics of PBX explosives, and also to determine the parameters of the model and to construct the damage evolution.

The K&C model considers that the damage evolution of the material mainly depends on the plastic strain in the material. Hence, the stress-(plastic strain) response (see Figure 4) of the material is analyzed. The elastic portion of the stress-strain curves was removed by the initial moduli of the curves.

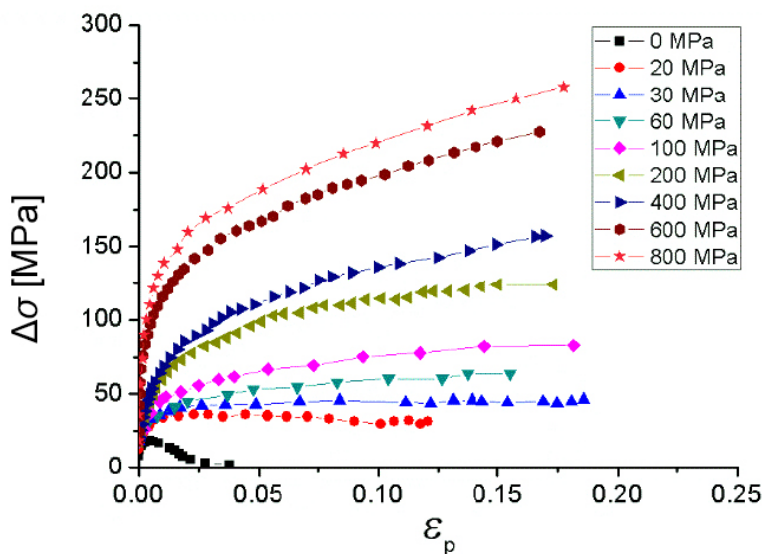


Figure 4. Stress-(plastic strain) curves of a PBX explosive under different confining pressures, obtained from test data in the literature [2]

The stress-(plastic strain) curves show that when the confining pressure is below the brittle-to-ductile transition pressure, the maximum stress value can be visible during the compression. However, when the confining pressure is greater than the brittle-to-ductile transition pressure, the stress will increase as the plastic strain increases. The maximum stress is not visible. In this case, the maximum stress in the model needs to be redefined. In order to solve this problem, it is necessary to analyze the stress-(plastic strain) response of the material under high pressures.

By analyzing the stress-(plastic strain) curves in Figure 4, it is found that the shape of the stress-(plastic strain) curves is similar to the shape of the compression meridians of the K&C model. Therefore, we constructed the following Equation 9 according to Equations 1-3. Equation 9 can be used to fit the data well when the pressure is greater than the brittle-to-ductile transition pressure:

$$\Delta\sigma = d + a\varepsilon_p + b\varepsilon_p/(1 + c\varepsilon_p) \quad (9)$$

where a , b , c and d are the parameters required to be optimized, ε_p is the plastic strain. In Equation 9, the unit of parameters a , b and d is MPa, and parameter c has no units. A comparison between the fitting curves and the test curves

is shown in Figure 5. The discrepancies between the fitting curves and the test curves are less than 5%. The fitting curves are in good agreement with the experimental curves. This demonstrates that Equation 9 can describe the stress-(plastic strain) responses of a PBX under high pressures. In other words, it can be expressed that when the pressure is greater than the brittle-to-ductile transition pressure, the stress-(plastic strain) response can be decomposed into linear and nonlinear terms (Equation 9). A similar understanding can also be obtained from the experimental data in the literature [16, 17]. The combination of the linear and non-linear responses may be a common characteristic of stress-(plastic strain), or stress-strain, responses of PBXs when the pressure is high. In the present paper, the linear term in Equation 9 is called the linear hardening portion, and the nonlinear term is called the nonlinear hardening portion. Figure 6 shows the variation of the fitting parameters a , b and c with different confining pressures p_a . Obviously, these variations do not show any pattern. This means that it is difficult to describe the stress-(plastic strain) response of PBXs by means of Equation 9 directly.

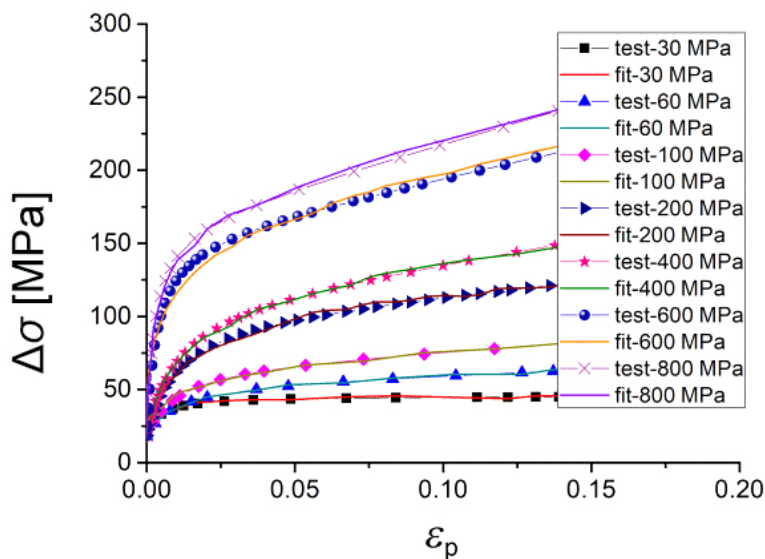
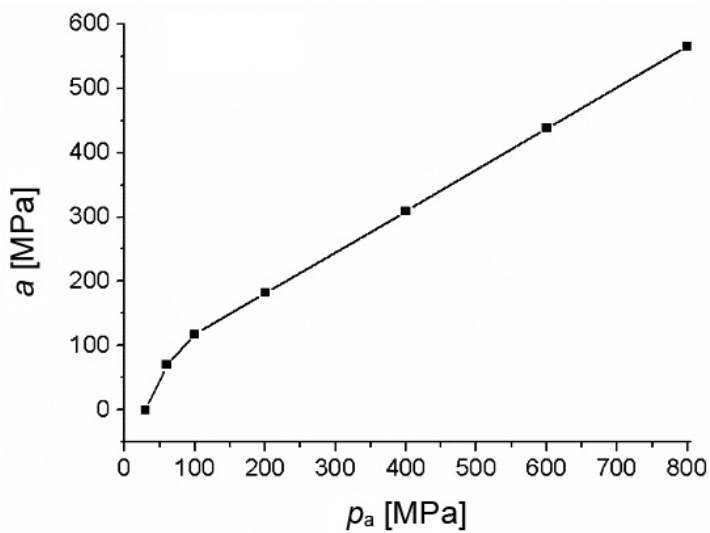
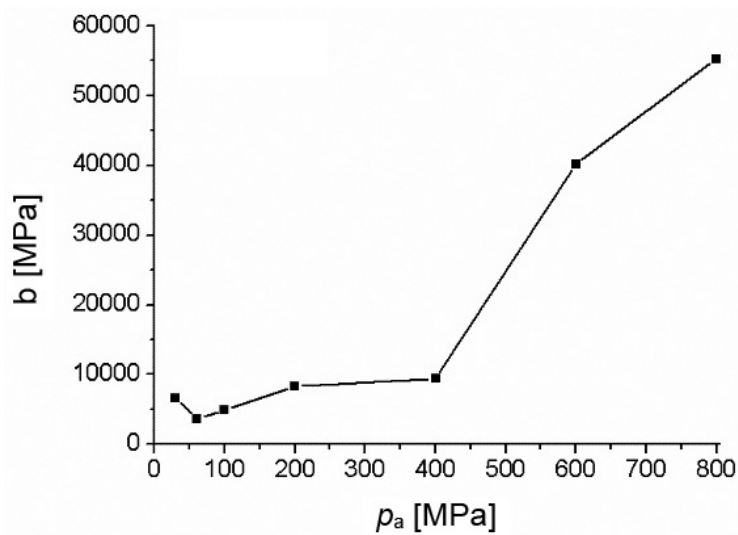


Figure 5. Comparison of stress-plastic strain test curves and fitting curves of PBXs under different confining pressures



(a)



(b)

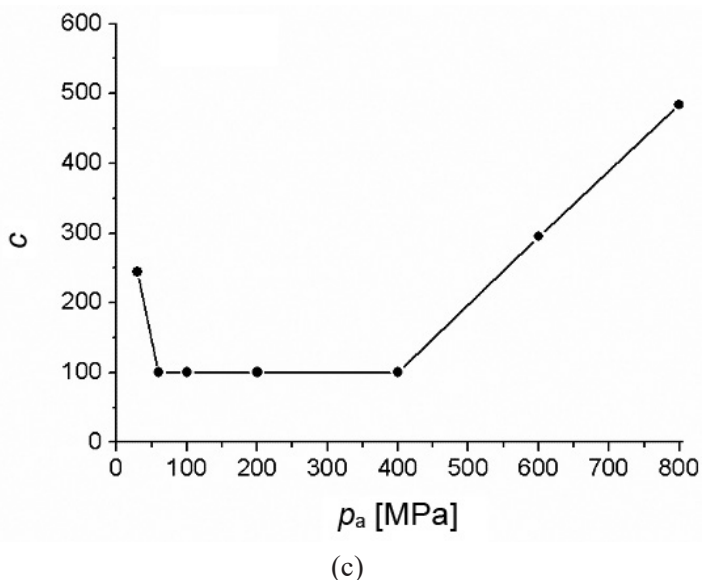


Figure 6. Variation of the fitting parameters with different confining pressures: parameter a (a), parameter b (b), and parameter c (c).

Figure 7 shows the sensitivity of the stress-plastic strain curve with respect to the parameters a , b and c . Parameters a , b and c were changed as follows: one of them was doubled while the others were kept unchanged. Note that the parameter d is only related to the initial value of the fitting curves, which is not analyzed. The result shows that the linear hardening portion of the curve is determined mainly by parameter a , while parameters b and c influence the nonlinear hardening portion of the curve. The change of the linear hardening portion (slope, parameter a) can be obtained from the experimental data directly, but the description of the nonlinear hardening portion needs to be considered by other methods, which are considered in the next section.

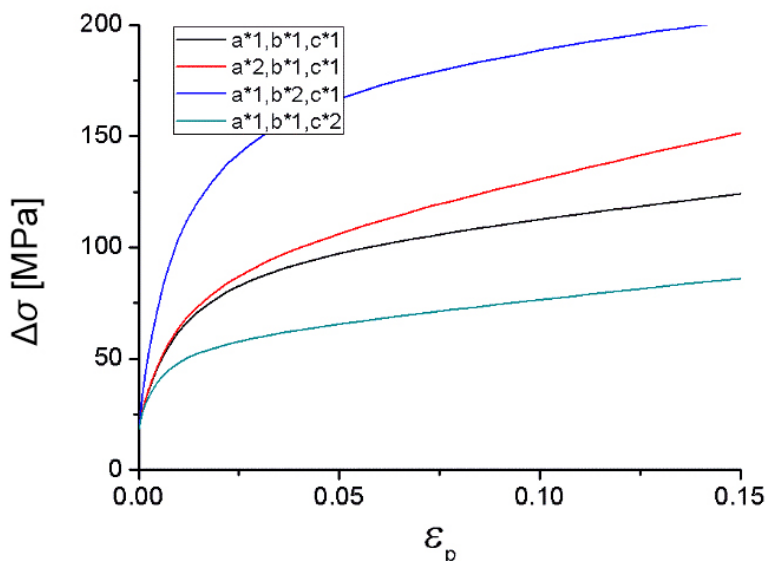


Figure 7. Sensitivity analysis of parameters a , b and c

It should be mentioned that the maximum stress commonly defined is the transition point between the nonlinear hardening portion and the softening portion. However, when the confining pressure is beyond the brittle-to-ductile transition pressure, the linear hardening portion appears instead of the softening portion. Therefore, the transition point between the non-linear hardening portion and the linear hardening portion can be defined as the maximum stress under high pressures, which is used to determine the parameters of the maximum strength surface in the K&C model. The maximum stress here is essentially the maximum value of the nonlinear hardening portion.

3 Implementation of the Model

3.1 Determination of the parameters

There are three strength surfaces in the model. The maximum strength surface can be determined from the experimental curves. Figure 8 shows the maximum strength of PBXs at different hydrostatic pressures.

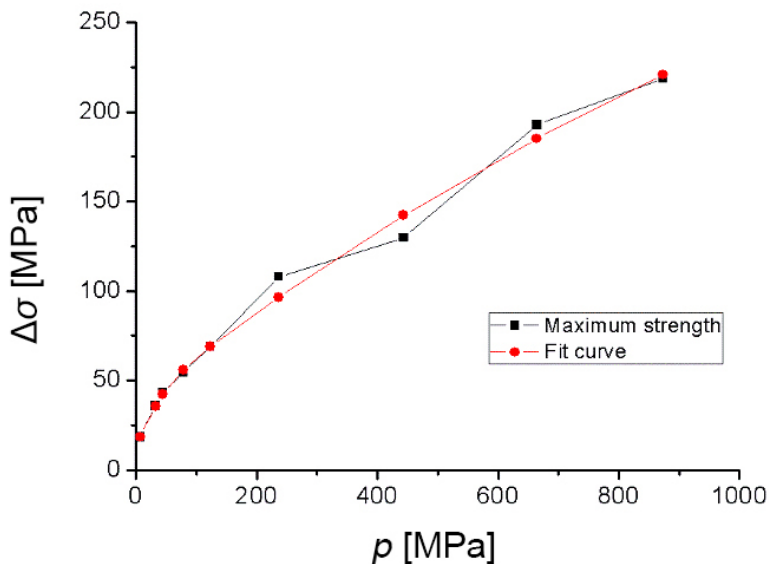


Figure 8. The maximum strength of a PBX

In order to conveniently determine the yield strength surface, the ratio between the yield strength and the maximum strength was considered to be 27.08% in this study, as shown in Figure 2 (along the interpolation path). The ratio 27.08% is based on the uniaxial compression test (18.46 MPa for uniaxial compressive strength f_c , 5 MPa for initial yield strength) [2]. This means that the parameters of the yield strength surface and the maximum strength surface are no longer independent. With the maximum strength surface parameters, the parameters of the yield strength surface can be directly determined from the ratio. This is a reference to the practice in the K&C model. In fact, it is not easy to accurately determine the yield strength point from the test data, and as an alternative a range which includes the accurate value is provided, especially when there is confining pressure.

There are two undetermined parameters in the residual strength surface (Equation 2), so the determination of the residual strength surface requires two constraints. One is the brittle-to-ductile transition condition, which is a meaningful physical constraint condition, and the other constraint is the softening portion of the stress-(plastic strain) curve at the confining pressure of 20 MPa. Actually, the softening part involves the structural failure of the material, so that it has a considerable uncertainty [22, 23]. Although describing the softening part is of importance for the assessment of structural damage, it is a complex problem beyond the scope of this study.

In order to achieve better characterization, the parameters of the strength surfaces are fitted in the two confining pressure ranges, of greater than and less than 100 MPa, and the fitting parameters are listed in Table 1. p_a in Table 1 is the confining pressure. The PBXs will not be softened under high confining pressure, so there are no parameters for residual strength surface when p_a is greater than 100 MPa. In this study, when the confining pressure is greater than the brittle-to-ductile transition pressure, the residual strength is equal to the maximum strength.

Table 1. Parameters of the strength surfaces

p_a [MPa]	a_0 [MPa]	a_1	a_2 [MPa ⁻¹]	a_{1f}	a_{2f} [MPa ⁻¹]	a_{0y} [MPa]	a_{1y}	a_{2y} [MPa ⁻¹]
≤100	13.298	1.1365	0.00891	5.903	-0.1278	4.527	3.46	0.03819
>100	36.387	3.625	0.00127	–	–	12.149	15.997	0.002997

The interpolation function (η - λ curve) connects the stress with the strain. This function is obtained based on the uniaxial compressive stress-(plastic strain) curve (see Figure 9). η is a normalized stress response (using uniaxial compressive strength) between the maximum strength and the yield strength (hardening process) or residual strength (softening process), and λ , as the damage parameter, is determined by the plastic strain (see Equation 8). The parameter b_1 takes 1.6, which is the default value in the K&C model of the LSDYNA software [24].

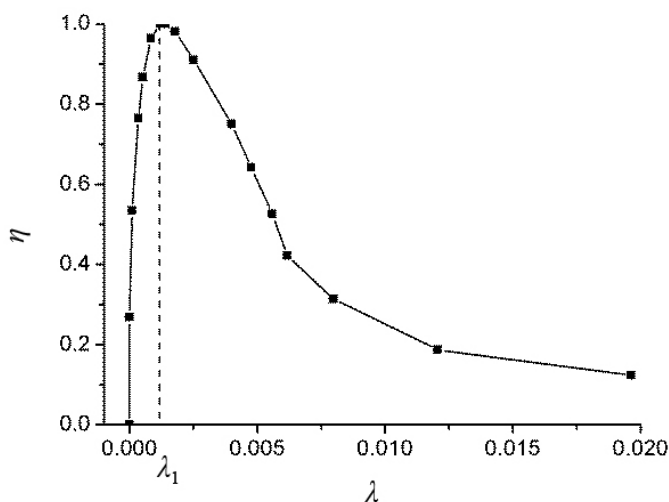


Figure 9. The interpolation function of the model

3.2 Determination of the current strength surface

In the K&C model, the current yield strength of the material depends on the interpolation between the maximum strength and the yield strength or the residual strength. At each time interval, the current yield strength could be computed according to the interpolation function (damage evolution curve) and the strength surfaces. This involves the choice of the interpolation path which is used for determining the values of strength surfaces (Equations 1-3). The actual loading path is difficult to judge because it may change at any time. It is not easy to use the actual loading path as the interpolation path. Studies of concrete materials have shown that different stress loading paths do not affect the maximum strength surface of the material [22]. Therefore, it is acceptable to use a fixed interpolation path to determine the current strength without considering the actual loading path. In the present study, the maximum strength and the yield strength (or residual strength) used for the interpolations are obtained by solving Equations 1-3, 10, and 11, then the current compression meridian is obtained by Equation 7. The Equations 10 and 11 are expressed as:

$$\eta(\lambda) = (p - p_x)/(p_m - p_x) \quad (10)$$

$$p = p_m - (1 - \eta(\lambda)) (\Delta\sigma_m - \Delta\sigma_x)/3 \quad (11)$$

where p_x is the hydrostatic pressure corresponding to the yield strength (p_y) or the residual strength (p_r), and $\Delta\sigma_x$ is the yield strength ($\Delta\sigma_y$) or the residual strength ($\Delta\sigma_r$), corresponding to the hardening section and the softening section, respectively.

The compression path (parallel to the uniaxial compression, in Figure 2) is adopted as the interpolation path, and Equations 10 and 11 are the mathematical representations of the compression path. It should be noted that the interpolation path is different from the loading path, and is only applied to the description of the current yield surface. At each cycle step, the hydrostatic pressure (p) and the interpolation function ($\eta(\lambda)$) in Equations 10 and 11 are known, then the current yield strength is calculated.

3.3 Pressure dependence of the moduli

Vial *et al.* [18], found the moduli of a PBX clearly varied with the confining pressure. Figure 10 shows the moduli-(confining pressure) curves. These curves are based on the experimental data given in reference [18] and have been partially modified according to the stress-strain curves in reference [2]. In the model

implemented in the present study, the dependence of the moduli on the confining pressures is considered.

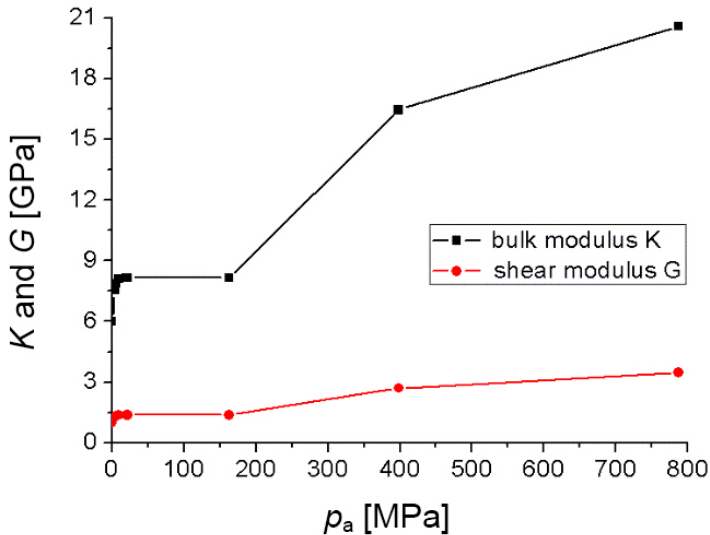


Figure 10. The variation of the moduli with confining pressure

In constitutive models, the hydrostatic pressure is often used to describe the pressure-dependent property of the material. However, if the elastic modulus of the material were expressed as a function of the hydrostatic pressure, with the hydrostatic pressure changing under axial compression, the elastic modulus of the material would also change, which is clearly unacceptable. In order to consider the linear hardening response under high pressures, the linear hardening modulus should remain unchanged during axial compression. Here, the confining pressure is used to describe the pressure-dependent property of the moduli. The confining pressure is obtained by subtracting the equivalent hydrostatic pressure from the hydrostatic pressure using the expression:

$$p_a = p - \sigma/3 \quad (12)$$

where p_a is the confining pressure, p is the hydrostatic pressure, and σ is the von Mises equivalent stress. This expression is based on the compression path (interpolation path). For the complex stress, this first needs to be transformed onto the compression path by Equation 5, followed by calculation of the confining pressure. For the complex stresses, the definition of confining pressure is an equivalent.

The variation of the linear hardening modulus with the confining pressure is shown in Figure 11; the data are taken from the experimental curves shown in Figure 3. According to the experimental data, the expression of the linear hardening modulus is written as Equation 13. The brittle-to-ductile transition pressure of the material was estimated to be 25.416 MPa.

$$\begin{cases} E_h = 0.544p_a + 115.352 & p_a \geq 80.179 \\ E_h = 2.903p_a - 73.791 & 80.179 > p_a \geq 0 \end{cases} \quad (13)$$

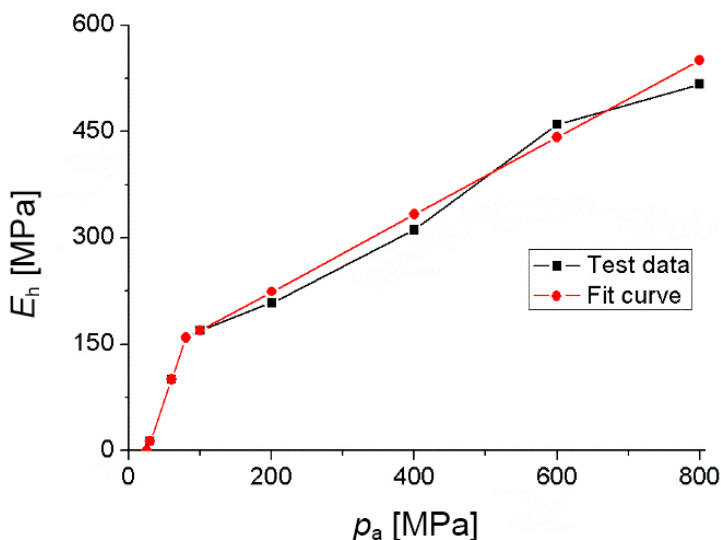
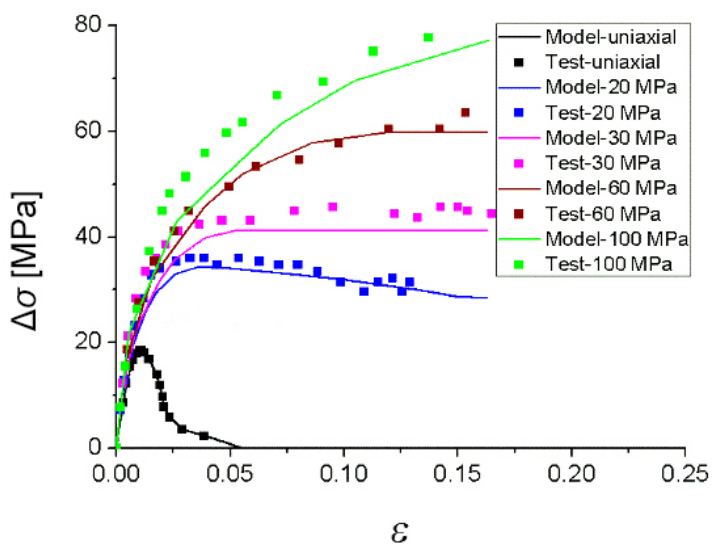


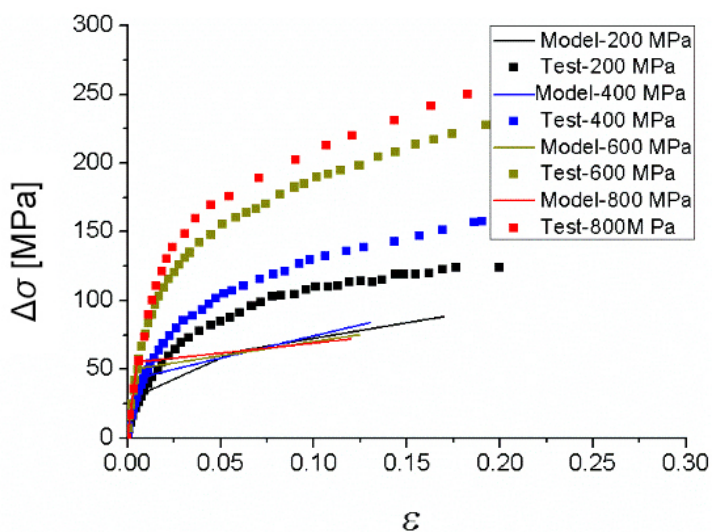
Figure 11. Variation of the linear hardening modulus with confining pressure

3.4 K&C model implementation in AUTODYN

In order to examine the ability of the K&C model to characterize the stress-strain responses of the material, a single element is used to compute the compression under different confining pressures. Implementation of the constitutive model was based on the secondary development of AUTODYN 17.0 [25]. In these computations, quasi-static compression is initially applied to produce the confining pressure, and then the velocity and fixed displacement boundary conditions are imposed at the top and bottom surfaces of the element respectively, after the hydrostatic pressure in the element has stabilized. A comparison between the calculated results and the experimental results is shown in Figure 12.



(a)



(b)

Figure 12. Comparison of experimental and simulation results using the original K&C model: confining pressure below (a) and above (b) 200 MPa.

The comparison shows that the K&C model is able to describe the variation of the stress-strain responses with confining pressures lower than 100 MPa (see

Figure 12(a)). However, when the stress reaches the maximum strength, the model cannot describe the hardening behaviour of the PBXs, which is an inherent limitation of the K&C model. In addition, under high confining pressures, the model calculation results are obviously underestimated compared with the test results, as is shown in Figure 12(b). This is due to the too slow growth of the damage parameter λ . This means that Equation 8 overestimates the influence of the hydrostatic pressure on damage evolution under high confining pressures.

3.5 Modified model

The shortcomings of the K&C model can be attributed to the limitation of its damage evolution curve. In the damage evolution curve, the K&C model does not consider the linear hardening state when the confining pressure is greater than the brittle-to-ductile transition pressure, and Equation 8 does not estimate the damage evolution process well.

In order to add the linear hardening state to the damage evolution curve, the damage parameter λ in the K&C model was modified. When the damage parameter λ is greater than λ_1 depending on the confining pressure, the material would present a hardening or softening state. The softening process is related to macroscopic cracks, but these macroscopic cracks would not appear in the hardening process under high confining pressures [13]. Thus two different damage parameter estimations are required to describe the two different processes respectively.

According to experimental observation of the meso-mechanism [2], the damage η is decomposed into the high pressure induced intragranular damage (η_{ID}) and the low pressure induced transgranular damage (η_{TD}), related to the parameters λ_{ID} and λ_{TD} , respectively. η_{ID} and η_{TD} are used to describe the hardening (both nonlinear and linear) and the softening behaviours, respectively. Under a confining pressure below the brittle-to-ductile transition pressure, the parameter λ_{ID} evolves and approaches λ_1 , while η_{ID} reaches 1 and then remains unchanged; η_{TD} is activated, and the corresponding parameter λ_{TD} begins to evolve. Under confining pressures greater than the brittle-to-ductile transition pressure, for the intragranular damage the parameter λ_{ID} evolves and approaches λ_1 , while η_{ID} reaches 1 and then remains unchanged; and the parameter λ_{ID} evolves further, leading to the stress increased with a hardening modulus (see Equation 13). The incremental expression of the damage parameters λ_{ID} and λ_{TD} are defined as:

$$\begin{cases} d\lambda_{TD} = d\lambda(1 - \Delta\sigma_r/\Delta\sigma_m) & \lambda > \lambda_1 \\ d\lambda_{ID} = d\lambda \Delta\sigma_r/\Delta\sigma_m & \lambda > \lambda_1 \\ d\lambda_{ID} = d\lambda & \lambda \leq \lambda_1 \end{cases} \quad (14)$$

These definitions ensure that the transgranular damage evolution parameter λ_{TD} can be gradually reduced to zero as the confining pressure is increased.

As described above, the damage evolution equation in the K&C model is not able to describe the damage evolution process correctly under high confining pressures. The main reason for this is that the effect of pressure on damage evolution is overestimated. In essence, the damage parameter λ (see Equation 8) is a normalized treatment of plastic strain produced under different confining pressures. The normalized characteristic value is the maximum failure strain corresponding to the maximum stress. This is explained directly in the RHT model, and the method is widely used in concrete models. Furthermore, the damage evolution parameter in the model is modified and expressed as:

$$\lambda = \int_0^{\varepsilon_p} d\varepsilon_p / (R_{DIF} \varepsilon_{\max}) \quad (15)$$

where ε_{\max} is the maximum failure strain under different confining pressures, and the other variables are consistent with those defined in Equation 8. Within a wide range of confining pressures, it is not easy to express the maximum failure strain as a function of the hydrostatic pressure. For simplicity, the maximum failure strain is expressed as a function of the confining pressure. This function is fitted directly from the experimental data and displays a bilinear function. It should be noted that the experimental data of the maximum failure strains given in Figure 13 are the minimum values, which can be considered as the transition point of the nonlinear and linear hardening sections in each experimental curve. Thus, increasing the value of the maximum failure strains here does not violate the definition of the maximum failure strength in this paper, but it should not be reduced. Since the transition point of the nonlinear hardening section and the linear hardening section is not obvious in the stress-strain curve given in the test when the confining pressure is greater than the brittle-to-ductile transition pressure, the maximum strength defined herein is actually a range rather than a specific value. This is good for the fitting, as shown in Figure 13, where some of the maximum failure strains are properly adjusted to satisfy the bilinear relationship (increasing their value). Note that the fitting here does not make the test data smaller because the test data have been obtained at a minimum.

The expressions of ε_{\max} fitted in Figure 13 are:

$$\begin{cases} \varepsilon_{\max} = 0.00004553p_a + 0.04907 & p_a \geq 31.2855 \\ \varepsilon_{\max} = 0.00149p_a + 0.003879 & 31.2855 > p_a \geq 0 \end{cases} \quad (16)$$

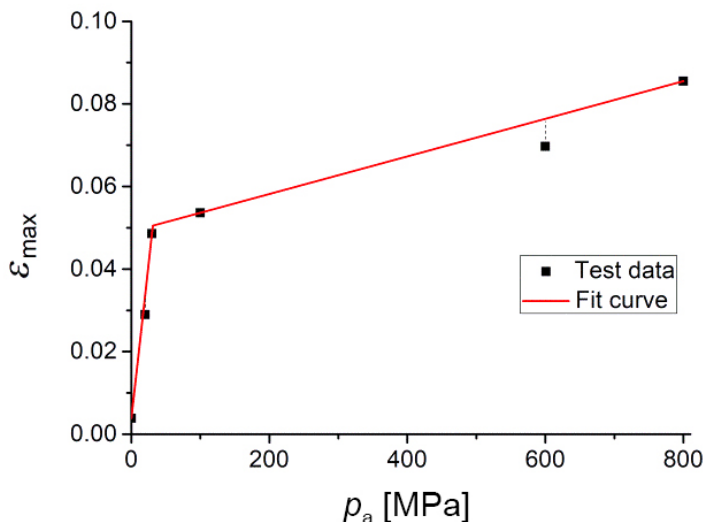


Figure 13. Variation of maximum failure strain with confining pressure

The fitting of the experimental data in Section 3 shows that the stress-(plastic strain) curves of PBXs are able to be expressed as a superposition of a linear term and a nonlinear term when the confining pressure is larger than the brittle-to-ductile transition pressure. The linear term can be obtained by fitting the experimental data (mainly the modulus, Equation 13), while the nonlinear term is difficult to describe due to the absence of obvious rules for the variation of the fitting parameters. According to the definition of the maximum strength in this study, the nonlinear term mainly describes the nonlinear hardening portion before the stress reaches the maximum strength. The damage evolution curve of the K&C model can be used to describe the nonlinear term. In order to describe the complete stress-strain response of materials under high confining pressures, the linear and nonlinear terms need to be considered together. Here, when the slope of the stress-(plastic strain) curve is reduced to the linear slope (see Equation 13), the linear function is used directly to describe the stress-(plastic strain) curve, otherwise, the linear function and the damage evolution curve in the K&C model are added together directly to describe the stress-(plastic strain) curve, and the expression is:

$$\eta_n(\lambda) = \max(1, \eta(\lambda)(1 - E_h \varepsilon_{\max} / ((1 - 0.2708)Y_{\text{MAX}})) + \lambda E_h \varepsilon_{\max} / ((1 - 0.2708)Y_{\text{MAX}})) \quad (17)$$

where $\eta(\lambda)$ is the original interpolation parameter in the original K&C model, and $\eta_n(\lambda)$ is a new interpolation parameter formed considering the linear term and the damage evolution. When $\eta_n(\lambda)$ is greater than 1, then set it to 1. Y_{MAX} is the maximum strength of the material estimated on the compression path (based on the known confining pressure), and can be expressed by Equations 18 and 19, respectively:

$$Y_{\text{MAX}} = 3(p_m - p_a) \quad (18)$$

$$Y_{\text{MAX}} = a_0 + p_m / (a_1 + a_2 p_m) \quad (19)$$

Equation 17 means that the proportion of the linear term in the nonlinear hardening part is calculated first, and then the interpolation parameter in the original K&C model is reduced according to the proportion. This method ensures that when the damage parameter λ reaches λ_1 , the new interpolation parameter $\eta_n(\lambda)$ is exactly 1. The flow chart of the modified constitutive model is shown in Figure 14. p_{btd} in the flow chart is the brittle-to-ductile transition pressure.

Here, the robustness of the model is also verified. So the parameters of the modified model are determined by using part of the test curves, and then the robustness of the model is verified by calculating the unused test curves. Parameters are determined in the same way as in the above sections.

The model proposed in this paper requires at least six test curves under different confining pressures to determine the parameters. Three test curves are for the confining pressure not below the brittle-to-ductile transition pressure; the other three are for confining pressure higher than the transition pressure. The uniaxial compression stress-strain curve is required. In this work, the test data from references [2] and [16] were utilized to verify the model.

The confining pressure conditions 20, 30, 100, 600 and 800 MPa were used to determine the parameters in the model. As Figure 15(a) shows, the stress-strain calculation results could match the test data well. Furthermore, using the calibrated parameters, the deformation under the confining pressure conditions 60, 200 and 400 MPa is predicted. In Figure 15(b), when the confining pressure is 400 MPa, there is an obvious difference between the calculation result and the experimental result. This difference contributes to the discreteness of the test data, with which the Equation 1 cannot be in agreement.

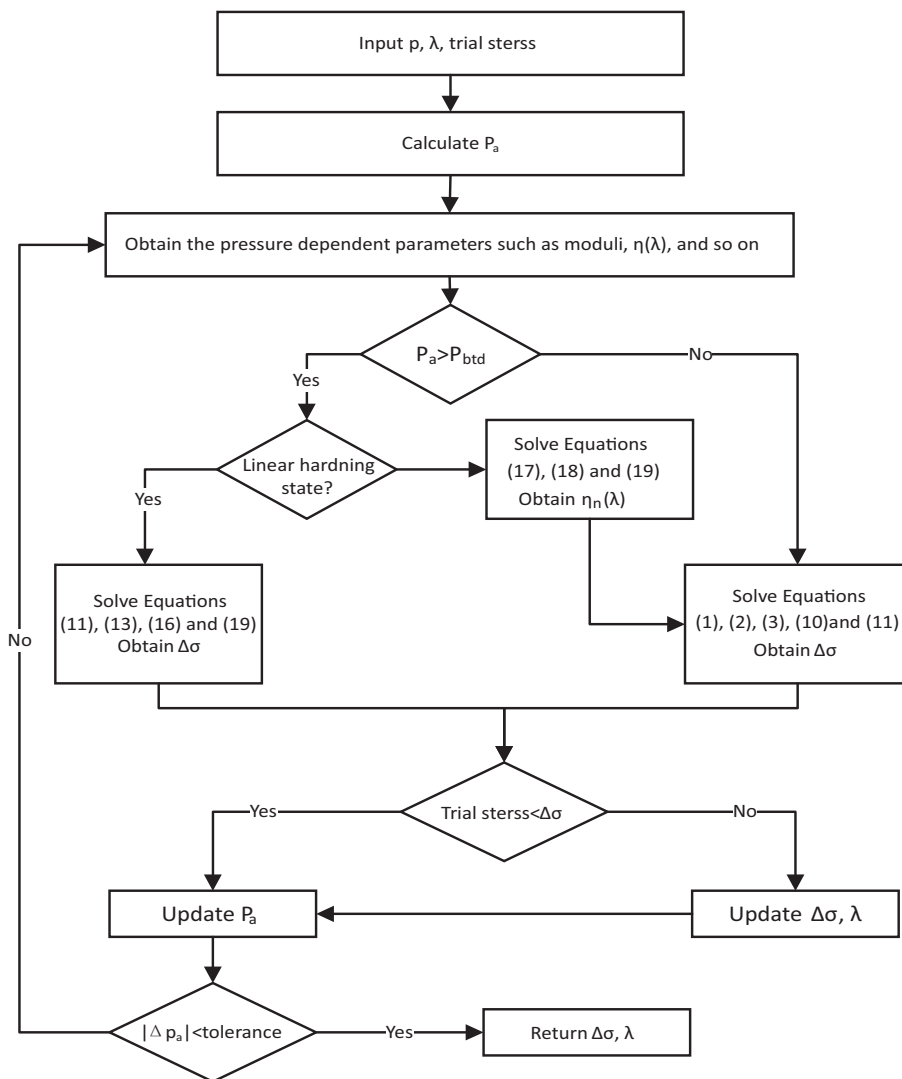
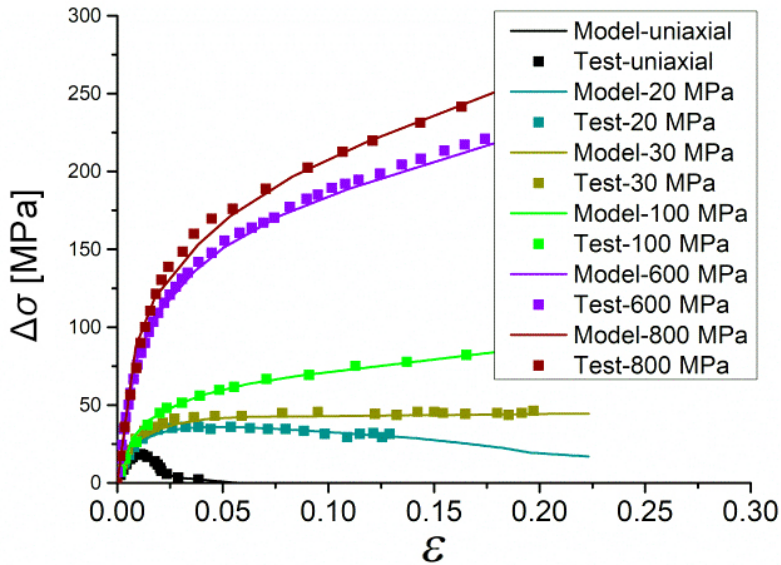
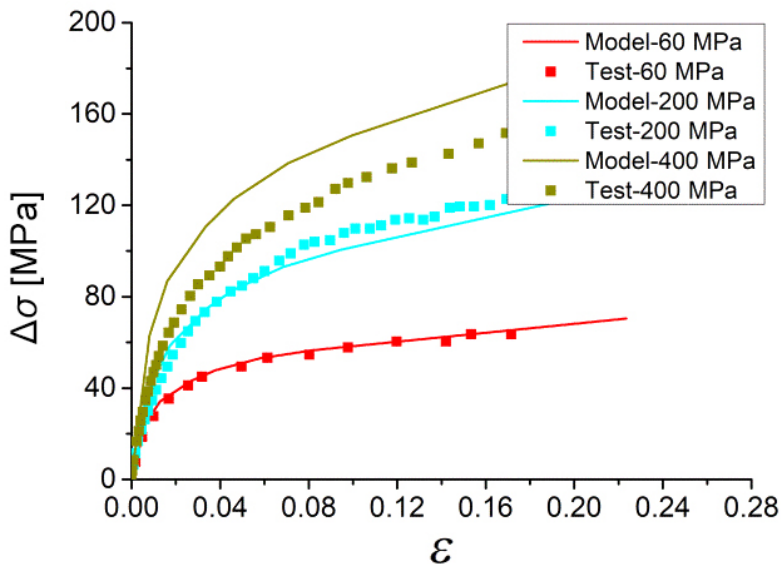


Figure 14. The flow chart of the modified constitutive model



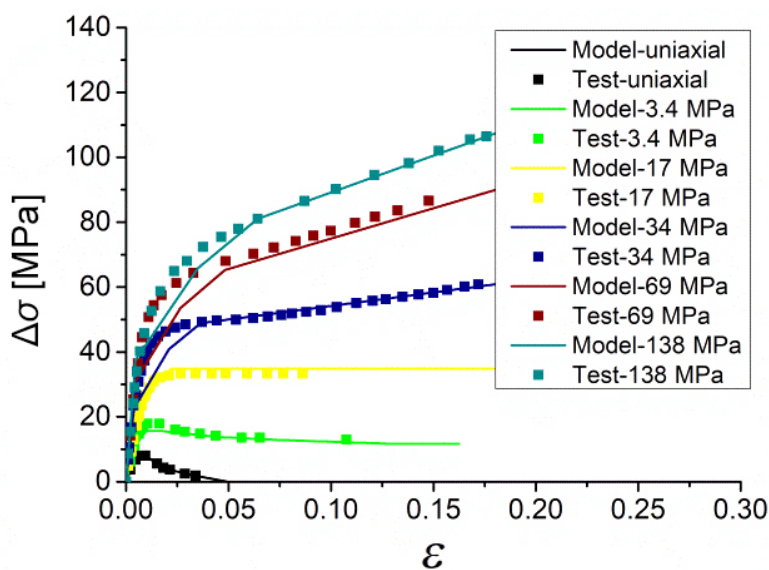
(a)



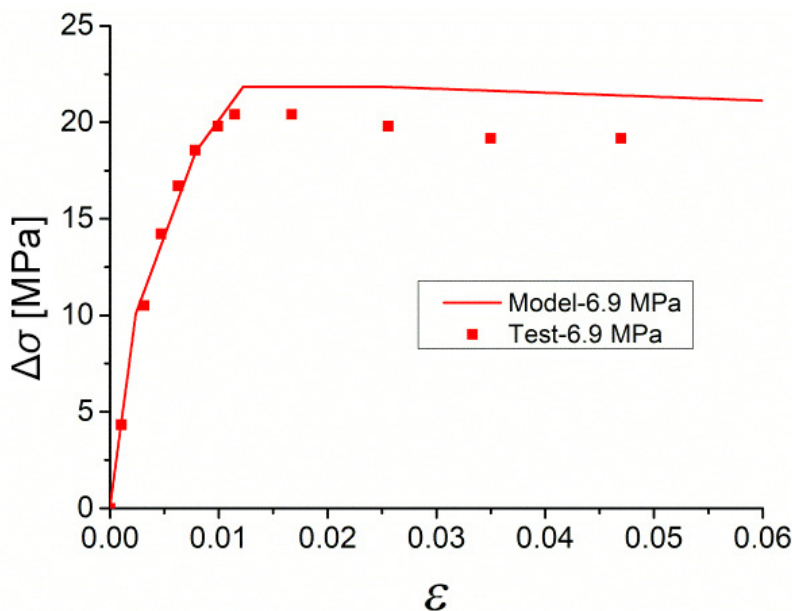
(b)

Figure 15. Comparison of experimental and calculation results using the modified K&C model (Test curves from [2]): stress-strain curves used to determine the parameters (a), and to verify the model (b)

Similarly, the model was verified for PBS 9501 described in [16], and its mechanical response behaviour is the same as that of PBX. As Figure 16(a) shows, the parameters in the model are calibrated well, and the stress-strain curves calculated match the test results under the confining pressure conditions of uniaxial compression, 3.4, 17, 34, 69 and 138 MPa. Figure 16(b) demonstrates that, by means of the model, the predicted result for the confining pressure of 6.9 MPa is comparable with the test result. Thus, the modified K&C model could be applied to predict the mechanical behaviour of PBXs, and the model has good robustness.



(a)



(b)

Figure 16. Comparison of experimental and calculation results using the modified K&C model (Test curves from [16]): stress-strain curves used to determine the parameters (a), and to verify the model (b)

4 Conclusions

- ◆ The K&C model was created based on a large number of experimental data. The model characterizes the stress-strain curves under different stress states by applying three key points combined with the damage evolution. In the present study, the modelling of the mechanical behaviour of constrained PBXs has been completed by means of using the framework of the K&C model with modified damage evolution. The main conclusions of this study are as follows:
- ◆ Under a confining pressure higher than the brittle-to-ductile transition pressure, $\Delta\sigma$ of PBXs can be expressed as two terms: linear and non-linear. The linear term (see Equation 9) primarily influences the linear hardening portion of the stress-(plastic strain) curve, and the nonlinear term influences the linear hardening portion. From this statement, the transition point of the nonlinear hardening portion to the linear hardening portion in the stress-(plastic strain)

curve can be defined as the maximum strength at high confining pressure, which is applied to determine the parameters of the maximum strength surface in the K&C model.

- ◆ The moduli of PBXs show significant pressure dependence. The elastic modulus or the linear hardening modulus will change with the hydrostatic pressure under uniaxial compression if it is expressed as a function of the hydrostatic pressure. This is unacceptable in our model. In order to consider the pressure-dependent properties of the moduli, a confining pressure is proposed, which is obtained by subtracting the equivalent hydrostatic pressure from the hydrostatic pressure. In addition, the confining pressure is applied for the correction of the damage evolution of the original K&C model (the estimation of the maximum strength in Equations 18 and 19).
- ◆ The original K&C model can describe the variation of the stress–strain response with confining pressures lower than 100 MPa. When the confining pressure is further increased, there will be a large deviation between the simulation and the experimental, which is due to the fact that significant linear hardening characteristics under high confining pressure are not considered in the original K&C model. In addition, the damage evolution in the original K&C model is too slow under high confining pressures, which is also the reason for the significant deviation. In order to solve these problems, a damage evolution equation was proposed. The damage is decomposed into transgranular damage and intragranular damage in the modified model. The transgranular damage is used to describe the softening behaviour of PBXs under low confining pressures, while the intragranular damage is used to describe the linear hardening behaviour of PBXs under the high confining pressures, which is not included in the original K&C model. Furthermore, the damage parameter λ is modified, and is more convenient for determining parameters from tests. A comparison between the simulation and the experimental results showed that the modified model can well describe the mechanical response of PBXs under different confining pressures.
- ◆ The method presented in this study is not limited to PBXs. Generally speaking, any materials that behave as Equation 9 can be described using this method.

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