

**A Pressure-Dependent Damage Model for Energetic
Materials**

by Joel B. Stewart

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A reprint from the JANNAF 45th Combustion / 33rd Airbreathing Propulsion / 33rd Exhaust Plume and Signatures / 27th Propulsion Systems Hazards Joint Subcommittee Meeting; Chemical Propulsion Analysis Center: Columbia, MD, December 2012.

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A PRESSURE-DEPENDENT DAMAGE MODEL FOR ENERGETIC MATERIALS

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ABSTRACT

Sub-detonative events occur when the explosive material in an energetic system reacts without fully detonating; for example, mechanical insult of an energetic system can result in either an explosion or deflagration, with much of the explosive either unreacted or burning. Despite this lack of detonation, the energetic response can still be quite violent and present safety issues to nearby systems and personnel. The investigation of sub-detonative response requires the consideration of an energetic material's mechanical strength because the plastic deformation and subsequent cracking of the energetic material influences both the reaction evolution (e.g., accelerated burn rate with increased surface area) and the level of violence in the response. In this paper, the kinematic homogenization approach of Hill and Mandel, a method that has been traditionally used in deriving yield criteria for void-metal aggregates, will be utilized in deriving a yield criterion for describing the mechanical response of energetic materials. The derived yield criterion is able to capture the strength-differential under constant pressure, which is expected in an energetic material, along with its dependence on both pressure and accumulated damage. The eventual goal is to be able to couple, in a consistent and physically-meaningful manner, the energetic material's mechanical response (through the yield criterion, appropriate damage nucleation and evolution laws, and the equation of state) with its reactive response.

INTRODUCTION

Explosions and deflagrations are classifications of sub-detonative high explosive responses that can occur when energetic systems are driven below the point of full detonation, yet still react (e.g., during mechanical insult). Even though the level of violence in these energetic responses is lower than for detonations, the outcomes are still hazardous to neighboring systems and personnel. A large amount of research has gone into characterizing the response of energetic systems that are driven to full detonation; however, much less work has been done on understanding and predicting sub-detonative responses.

The investigation of sub-detonative response requires the consideration of the mechanical strength of energetic materials [1,2,3]. This consideration is necessary because the plastic deformation and subsequent cracking of the energetic material influences the reaction evolution (e.g., accelerated burn rate with increased surface area) and the level of violence in the response. The mechanical strength of energetic materials is an area of research that has not been heavily investigated. The main reasons for this lack of research seem to be 1) mechanical strength of energetic materials is of negligible importance during full detonation (the type of energetic response for which most systems are designed) and 2) experimental characterization of energetic mechanical strength is challenging due to the material's pressure-dependent behavior and the justified fear experimentalists have of ruining expensive equipment if the energetic sample reacts violently.

In this paper, the kinematic homogenization approach of Hill and Mandel [4,5] will be used to derive a pressure-dependent model that can describe the mechanical response of damaged energetic materials. The yield criterion developed in the following sections is meant to describe the behavior of a binder-crystal-void energetic aggregate, where the void-free material (i.e., the binder-crystal aggregate) is termed the matrix material. Energetic materials typically display pressure-dependent strength behavior and initially contain both voids (due to

manufacturing) and grain surfaces, with new voids and surfaces potentially nucleating during loading. The desired properties of the overall yield criterion are as follows:

- 1) pressure-dependent matrix (this eliminates as potential candidates most metallic material models);
- 2) tension-compression asymmetry in the matrix material, even under constant pressure (this eliminates as potential candidates Drucker-Prager, Mises-Schleicher, etc.); and
- 3) damage that occurs due to both void evolution and new grain surface formation (from cracking of existing grains).

One possibility for capturing the damage in the explosive material is to derive an expression accounting for the void-based damage first, and then to introduce the more brittle grain-cracking damage through an appropriate nucleation and/or evolution law, thus, accounting for the third desired property listed previously. Nucleation and/or evolution laws for brittle damage is not the focus of this paper, but the first step—in other words, the incorporation of void-based damage to obtain a criterion describing the response of the binder-crystal-void aggregate—will be investigated in the following sections. The eventual goal is to be able to couple, in a consistent and physically-meaningful manner, the energetic material's mechanical response (through the yield criterion, damage evolution and equation of state) with its reactive response.

DAMAGE-FREE YIELD CRITERION

Prior to considering the influence of damage on the mechanical response of the energetic material, a yield criterion that describes the undamaged material (i.e., the binder and energetic crystals mixture) must first be identified. In order to capture the desired properties 1) and 2) listed in the previous section for the energetic material's yield criterion, let the yield criterion for the undamaged binder-crystal mixture be described as follows:

$$F = \sqrt{3J_2} - \frac{(3\alpha P_s + \kappa)}{g(\theta)} = 0, \quad (1)$$

where α and κ are material parameters, P_s is the pressure in the solid material ($P_s = -\sigma_{kk}/3$) and $J_2 = s_{ij}s_{ij}/2$ is the second invariant of the stress deviator, \underline{s} . The function, $g(\theta)$, introduces a dependence on the Lode angle, θ , and is assumed to be given as

$$g(\theta) = \cos \left[\beta \frac{\pi}{6} - \frac{1}{3} \cos^{-1}(\gamma \cos 3\theta) \right], \quad (2)$$

where β and γ are material parameters (assumed constant) that dictate the shape of the yield surface in the octahedral plane (see Figure 1). The Lode angle dependence of Eq. (2) was taken to be of the form shown in [6]. The Lode angle, θ , is typically defined as

$$\theta = \frac{1}{3} \cos^{-1} \left(\frac{3\sqrt{3}}{2} \frac{J_3}{J_2^{3/2}} \right), \quad (3)$$

where $J_3 = s_1s_2s_3$ is the third invariant of the stress deviator with s_i being the principal values of the stress deviator, \underline{s} . Note that for $\beta = 1$ and $\gamma = 0$, $g(\theta) = 1$ such that the matrix yield criterion reduces to the Drucker-Prager criterion (see Eqs. (1) and (2)).

The criterion describing the yield behavior of the undamaged energetic material (see Eqs. (1) through (3)) has four material parameters. The parameters α (non-dimensional) and κ (units of stress) control the slope and intercept, respectively, in the meridional plane, while β and γ (both non-dimensional) control the shape in the octahedral plane. These four parameters

would need to be determined experimentally for a given material. If the uniaxial yield strengths in tension and compression (σ_T and σ_C , respectively) are known, the meridional parameters α and κ can be determined as

$$\alpha = \frac{g_C \sigma_C - g_T \sigma_T}{\sigma_C + \sigma_T} \quad (4)$$

and

$$\kappa = \sigma_T (g_T + \alpha), \quad (5)$$

where $g_T = g(\theta = 0)$ and $g_C = g(\theta = \pi/3)$ are determined from Eq. (2).

In Figure 1 is depicted the dependence of the shape of the yield surface (Eq. (1)) in the octahedral plane with the material parameters β and γ . The plots all use values of $\alpha = 0.164$ and $\kappa = 1.648$ MPa. Note that the dependence of Eq. (1) on the Lode angle (see Eq. (2)) yields quite general shapes and is able to handle a large range of material yield responses. For energetic materials, the main desire was to be able to capture different yield strengths in tension versus compression at fixed pressures, which the form of Eq. (2) obviously allows (see, for example, Figures 1b through 1d).

In Figure 2 is illustrated the criterion given by Eq. (1) in the meridional plane. Note that the profile shown is similar to what would be obtained by a Drucker-Prager criterion since $g(\theta)$ simply controls the shape in the octahedral plane. Similar to Figure 1, the curve shown in Figure 2 was generated for values of $\alpha = 0.164$ and $\kappa = 1.648$ MPa.

Figure 3 displays the yield surface in rotated 3D principal stress space (rotated such that the (1,1,1) vector, the vector corresponding to the hydrostatic axis, is now the 3-direction). This space is a combination of Figures 1 and 2 (i.e., horizontal slices are the octahedral profiles while vertical slices are the meridional profiles). Note that the surface results in an infinite geometry for compressive pressures (similar to a Drucker-Prager or Mises-Schleicher criterion, for example).

The criterion of Eq. (1) predicts an infinite yield strength in hydrostatic compression, an undesirable result that is typically resolved in the geomaterials community (who also must deal with pressure-dependent yield surfaces) by assuming a “cap” function that describes the material behavior at high compressive pressures (this cap may harden with, for example, plastic work). In this work, the issue of an infinite yield strength with increasing compression will be resolved by looking at the influence of damage; this damage may be due to either voids or, more dominant at high compressive pressures, cracking crystals that generate new surfaces.

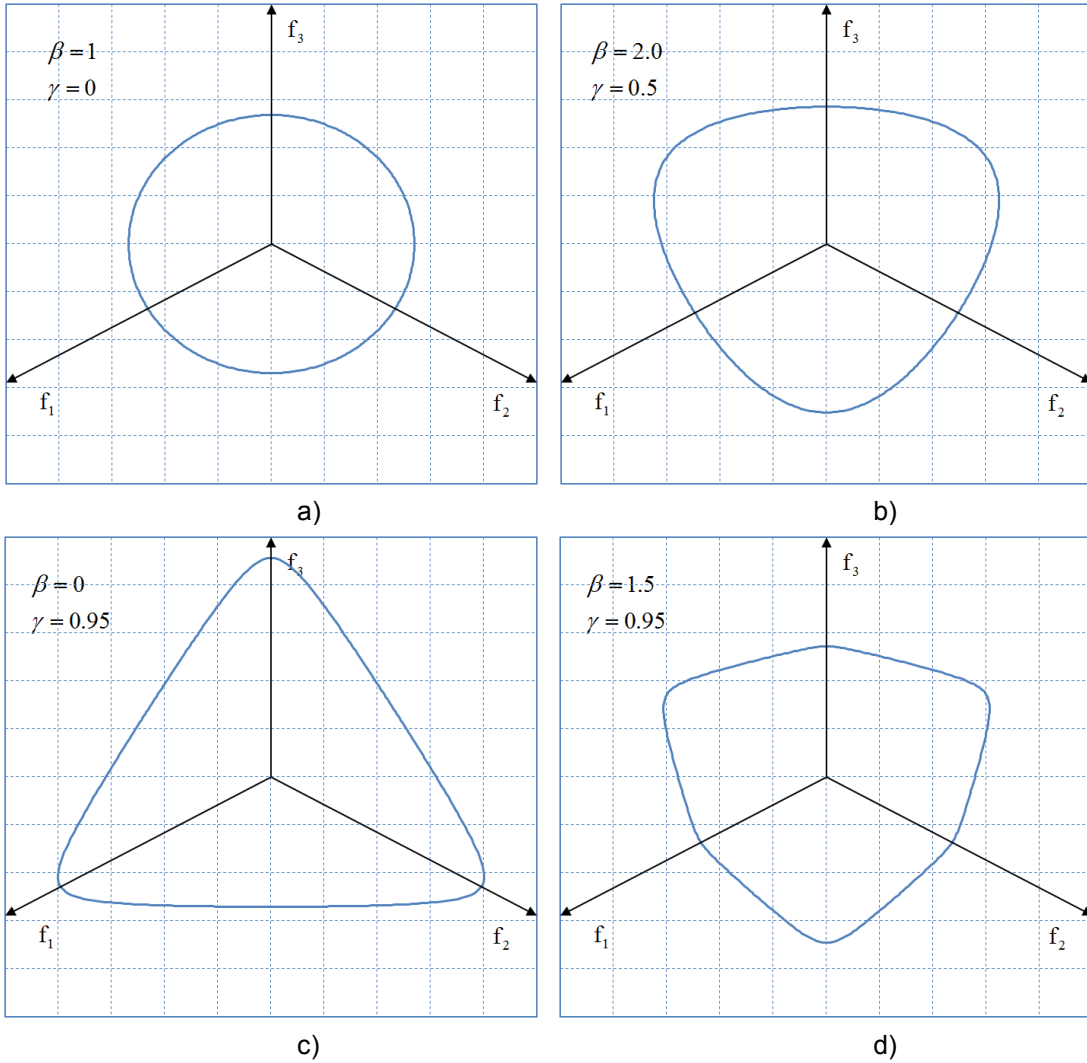


Figure 1: Undamaged yield criterion of Eqs. (1) and (2) plotted in the octahedral plane (and assuming $P=0$) with $\alpha = 0.164$, $\kappa = 1.648$ MPa and a) $\beta = 1$, $\gamma = 0$; b) $\beta = 2.0$, $\gamma = 0.5$; c) $\beta = 0$, $\gamma = 0.95$; d) $\beta = 1.5$, $\gamma = 0.95$.

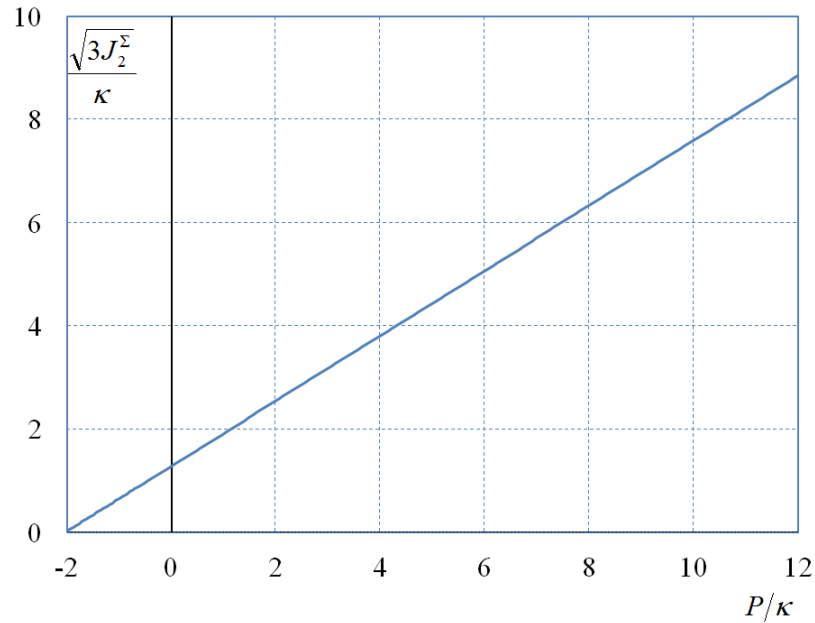


Figure 2: Undamaged yield criterion of Eqs. (1) and (2) plotted in the meridional plane for a fixed Lode angle ($\theta = 0$) with $\alpha = 0.164$ and $\kappa = 1.648$ MPa.

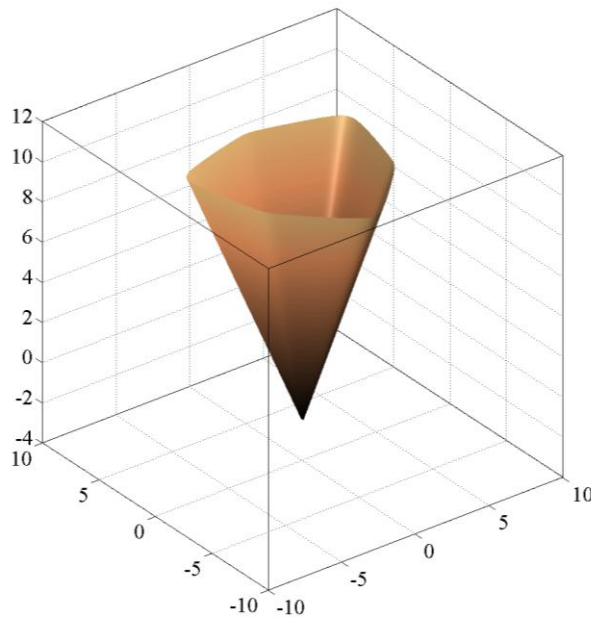


Figure 3: Undamaged yield criterion of Eqs. (1) and (2) plotted in 3D (rotated) principal stress space for $\alpha = 0.164$, $\kappa = 1.648$ MPa, $\beta = 1.5$ and $\gamma = 0.95$.

HYDROSTATIC LOADING CONDITION

Given a spherical representative volume element (RVE) containing a spherical void and obeying the yield condition of Eq. (1), an approximate solution for the limit pressure (i.e., the

pressure at which the entire sphere is plastic) may be obtained for the case of either tensile hydrostatic loading or compressive hydrostatic loading. The relevant equilibrium equation is

$$\frac{d\sigma_r}{dr} + 2\left(\frac{\sigma_r - \sigma_\theta}{r}\right) = 0, \quad (6)$$

with assumed boundary conditions of zero-traction on the void boundary ($r = a$),

$$\sigma_r = 0 \Big|_{r=a}, \quad (7)$$

and an applied pressure load on the outer surface ($r = b$),

$$\sigma_r = P \Big|_{r=b}. \quad (8)$$

From symmetry, the local stress tensor and its deviator can be written as

$$\underline{\sigma} = \begin{bmatrix} \sigma_r & 0 & 0 \\ 0 & \sigma_\theta & 0 \\ 0 & 0 & \sigma_\theta \end{bmatrix} \quad \text{and} \quad \underline{s} = \frac{\sigma_r - \sigma_\theta}{3} \begin{bmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (9)$$

The relevant local stress invariants are given as

$$P_s = -\frac{\sigma_r + 2\sigma_\theta}{3}, \quad (10)$$

$$J_2 = \frac{(\sigma_r - \sigma_\theta)^2}{3}, \quad (11)$$

and

$$J_3 = \frac{2}{27}(\sigma_r - \sigma_\theta)^3. \quad (12)$$

Hooke's law and strain compatibility can be combined with the equilibrium equation of Eq. (6) to determine an expression for the local stress field in the RVE. The details of this derivation will be omitted here since the focus of this paper is on macroscopic quantities. However, a result from this derivation that will be used in the following is a relationship between the local pressure in the elastic solid and the macroscopic pressure on the boundary of the RVE. This relationship is

$$P_s = \frac{P}{1-f}, \quad (13)$$

where $f = (a/b)^3$ is the void volume fraction. Note that, while the local pressure field in the elastic region of the sphere is constant, this is not necessarily the case for the local pressure field in the plastic region. However, in order to obtain an analytical expression for the limit pressure, the use of a constant, average pressure in the plastic region (assumed to be given by Eq. (13)) will be made when integrating Eq. (6).

It can also be shown from the local stress field that the sign of the applied macroscopic pressure is the same as the sign of the third invariant of the stress deviator given by Eq. (12). Note from Eqs. (2), (3), (11) and (12) that the Lode angle is constant throughout the RVE and given as

$$g_h = \begin{cases} g_r = g(\theta = 0) & \text{if } P > 0 \\ g_c = g\left(\theta = \frac{\pi}{3}\right) & \text{if } P < 0 \end{cases}, \quad (14)$$

where the fact that the sign of the applied macroscopic pressure is equal to the sign of the third invariant of the stress deviator has been used. Now, the matrix yield criterion of Eq. (1) can be combined with Eqs. (11), (14) and the equation of motion (Eq. (6)) to yield

$$P = \mp \frac{2}{3} \ln(f) \left(\frac{3\alpha P_s + \kappa}{g_h} \right). \quad (15)$$

Using Eq. (13), this result can be written as

$$P = \frac{\mp \frac{2}{3} \kappa \ln(f)}{g_h \pm \frac{2}{3} \left(\frac{3\alpha}{1-f} \right) \ln(f)} \quad (16)$$

such that the tensile limit pressure is

$$P_Y^+ = \frac{-\frac{2}{3} \kappa \ln(f)}{g_T + \frac{2}{3} \left(\frac{3\alpha}{1-f} \right) \ln(f)} \quad (17)$$

and the compressive yield pressure is

$$P_Y^- = \frac{\frac{2}{3} \kappa \ln(f)}{g_C - \frac{2}{3} \left(\frac{3\alpha}{1-f} \right) \ln(f)}. \quad (18)$$

Alternatively, Eq. (16) can be written as

$$\ln(f) = \mp \frac{3}{2} \left(\frac{P g_h}{\kappa + \frac{3\alpha P}{1-f}} \right). \quad (19)$$

This last equation is useful for comparing with the hydrostatic term derived in the next section for a damaged energetic material.

YIELD CRITERION FOR THE DAMAGED ENERGETIC MATERIAL

In this section, a yield criterion will be derived that combines the influence of the binder-crystal aggregate (see Eq. (1)) with that of voids. Even though damage due to voids would seem secondary to damage due to cracking of the explosive crystals, the result obtained in this section could eventually be generalized to include damage due to both voids and cracking (through, for example, an appropriate brittle damage nucleation and growth law). The Hill-Mandel homogenization technique will be used for this derivation—a procedure which has been used heavily in the metallic community to derive models for describing the ductile behavior of metals (see, for example, [7, 8, 9, 10]). The yield criterion describing the behavior of the binder-crystal mixture (see Eqs. (1) and (2)) is already somewhat complicated compared to, for example, the von Mises yield condition (this was the criterion used to describe the matrix material in Gurson's classical model [7]). However, the homogenization procedure using the Hill-Mandel lemma can be greatly simplified by assuming a non-associative flow rule (this assumption is widely made for geological material models), where the plastic potential, G , is assumed to coincide with the von Mises effective stress. In other words,

$$d_{ij} = \dot{\lambda} \frac{\partial G}{\partial \sigma_{ij}} \quad \text{with} \quad G = \sqrt{3J_2}, \quad (20)$$

where d_{ij} is the local rate of deformation tensor and σ_{ij} is the local Cauchy stress tensor. Using Eq. (20), the expression for the plastic multiplier, $\dot{\lambda}$, is shown to be as follows:

$$\dot{\lambda} = \sqrt{\frac{2}{3} d_{ij} d_{ij}}. \quad (21)$$

The derivation of a macroscopic yield criterion using Hill-Mandel's lemma proceeds similarly to what has been done before [8,9,10]. The following presents the key equations with some details omitted. Assume a velocity field of the form (see [11])

$$\underline{v} = \underline{v}^V + \underline{v}^S \quad (22)$$

with

$$\underline{v}^V = D_m \left(\frac{b^3}{r^2} \right) \underline{e}_r \quad \text{and} \quad \underline{v}^S = \underline{\underline{D}}' \underline{x}, \quad (23)$$

where \underline{e}_r and \underline{x} are unit vectors in the spherical coordinate system (radial direction) and Cartesian coordinate system, respectively, and b is the outer radius of the assumed spherical RVE containing a spherical void of radius a . Transforming everything to the spherical coordinate system, the components of the local rate of deformation tensor can be shown to be

$$d_{rr} = -2D_m \left(\frac{b}{r} \right)^3 + D'_{rr}, \quad (24a)$$

$$d_{\theta\theta} = D_m \left(\frac{b}{r} \right)^3 + D'_{\theta\theta}, \quad (24b)$$

$$d_{\phi\phi} = D_m \left(\frac{b}{r} \right)^3 + D'_{\phi\phi}, \quad (24c)$$

$$d_{r\theta} = D'_{r\theta}, \quad (24d)$$

such that

$$d_{ij} d_{ij} = \frac{3}{2} D_e^2 + 6 \left(\frac{D_m}{u} \right)^2 - 6 \frac{D_m}{u} D'_{rr}, \quad (25)$$

where $u = r^3/b^3$ and $D_e = \sqrt{(2/3) D'_{ij} D'_{ij}}$. Assuming that the local rate of deformation is purely inelastic, the local plastic dissipation, $w(\mathbf{d})$, can be written as

$$\begin{aligned} w &= \sigma_{ij} d_{ij} \\ &= \sigma_{ij} \dot{\lambda} \frac{\partial G}{\partial \sigma_{ij}} \\ &= \dot{\lambda} G, \\ &= \dot{\lambda} \left[\frac{3\alpha P_s + \kappa}{g(\theta)} \right], \end{aligned} \quad (26)$$

where $g(\theta)$ is given by Eq. (2). The Hill-Mandel lemma applies for the uniform strain rate boundary condition given by Eqs. (22) and (23). Thus, there exists an average plastic dissipation, $W(\mathbf{D})$, related to the average stresses, Σ_{ij} , as

$$\Sigma_{ij} = \frac{\partial W}{\partial D_{ij}}. \quad (27)$$

The average and local plastic dissipations are related through

$$W(\mathbf{D}) = \frac{1}{\Omega} \int_{\Omega-\omega} w(\mathbf{d}) dV . \quad (28)$$

Technically, Eq. (28) gives the expression for an upper bound to the true plastic dissipation in the representative volume element with volume Ω and containing a void of volume ω (because only the single kinematically admissible velocity field of Eqs. (22) and (23) is considered and there is no guarantee that this velocity field gives the infimum of the local plastic dissipation).

Equations (21), (24), (26), (27) and (28) can now be combined to determine expressions for the average stress invariants in the representative volume element and these expressions, in turn, can be combined to form the yield criterion for the void-matrix aggregate. In the interest of making it to the end of the derivation with an analytical form for the void-matrix criterion, the following assumptions will be made:

- A1) The local pressure in the solid, P_s , is related to the average pressure on the boundary, P , through $P = (1 - f)P_s$, where f is the void volume fraction. Note that this relationship coincides with the earlier assumption made in the simplified analysis of a hollow sphere loaded hydrostatically (see Eq. (13)).
- A2) The Lode angle, θ , in the matrix material is considered to be constant under the considered loading conditions of Eq. (23). This assumption can also be shown to hold for the simplified case of a hollow sphere loaded hydrostatically (see Eq. (14)).

Note that, if nothing else, using Assumptions A1) and A2) should recover the solutions obtained in the purely hydrostatic analysis (see Eq. (19)). The validity of these assumptions and the resulting yield criterion for general loading states will need to be further investigated.

A macroscopic criterion for the void-matrix aggregate (with the matrix material being the binder-crystal mixture obeying Eqs. (1) and (2)) can be derived using Eqs. (26) and (28) as well as Assumptions A1) and A2) and the Hill-Mandel lemma (see references [9] and [10] for a similar analysis). The resulting expression is

$$\Phi = \left(\frac{\sqrt{3J_2^\Sigma} g(\theta)}{\kappa + \frac{3\alpha P}{1-f}} \right)^2 + 2f \cosh \left(\frac{3Pg_h}{2 \left(\kappa + \frac{3\alpha P}{1-f} \right)} \right) - 1 - f^2 = 0 , \quad (29)$$

where f is the damage in the void-matrix aggregate (f is considered here to be a generalized damage variable since the goal is to eventually capture both void volume fraction and damage due to cracking) and g_h is the value of the Lode-angle function corresponding to the case of a hydrostatically-loaded hollow sphere (see Eq. (14)). The superscript on the second deviatoric stress invariant, J_2^Σ , denotes that this invariant is with respect to the average stresses, Σ_{ij} , and $g(\theta)$ is now assumed to be with respect to the average stress invariants. Note that Equation (29) reduces to Equation (1) if there is no damage in the material (i.e., if $f = 0$). Eq. (29) reduces to the hydrostatic solutions given by Eq. (19) when the deviatoric stresses vanish (i.e., when the first term in Eq. (29) is zero).

The deviatoric term (first term) in Eq. (29) uses the general expression for the Lode angle θ , which depends on the specific loading condition (as opposed to the hydrostatic term, or second term in Eq. (29), where θ is taken to correspond to either the tensile or compressive

hydrostatic case). However, the hydrostatic pressure relation of Eq. (13), relating the macroscopic (or average) pressure to the local pressure, is used in both the deviatoric and hydrostatic terms of Eq. (29). Perhaps a more suitable relation for the pressure relation in the deviatoric term could be determined, for example, by considering some purely deviatoric loading condition.

Figure 4 depicts Eq. (29) in the octahedral plane for both $f = 0$ (void-free) and $f = 0.25$. Note that the presence of damage tends to shrink the yield surface in the octahedral plane (i.e., the material loses its capacity to sustain shape-changing stresses). Figure 5 shows Eq. (29) in the meridional plane for various levels of damage. Note that in both Figures 4 and 5 the material's yield surface contracts as damage is accumulated. If damage is not allowed to accumulate during compression, the criterion of Eq. (29) will reduce to Eq. (1) at high pressures as all the voids are crushed out of the material (i.e., f will tend toward 0). Thus, damage due to cracking at high compressive pressures will need to be introduced into the damage evolution equation to avoid infinite yield strength at high compressive pressures. Finally, in Figure 6 is shown the yield surface of Eq. (29) in rotated 3D principal stress space (analogous to Figure 3) for $f = 0.20$ (each vertical slice is a meridional profile while each horizontal slice is an octahedral profile).

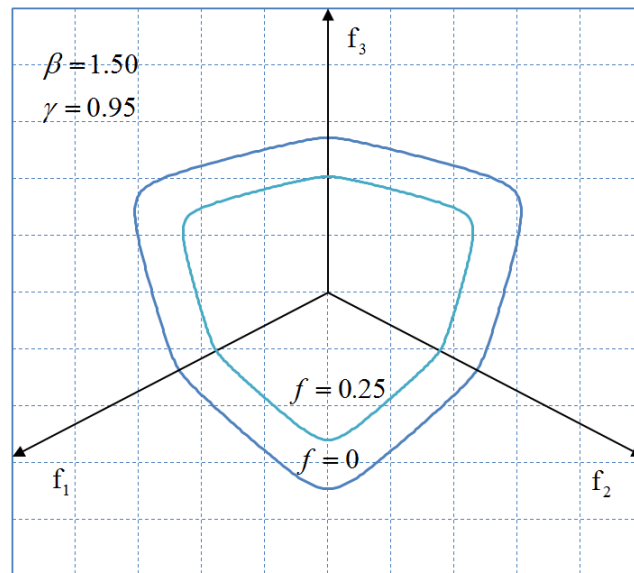


Figure 4: Yield criterion of Eq. (29) for the void-matrix aggregate plotted in the octahedral plane (and assuming $P = 0$) with $\alpha = 0.164$, $\kappa = 1.648$ MPa, $\beta = 1.5$ and $\gamma = 0.95$ for void volume fractions of $f = 0$. (i.e., void-free) and $f = 0.25$.

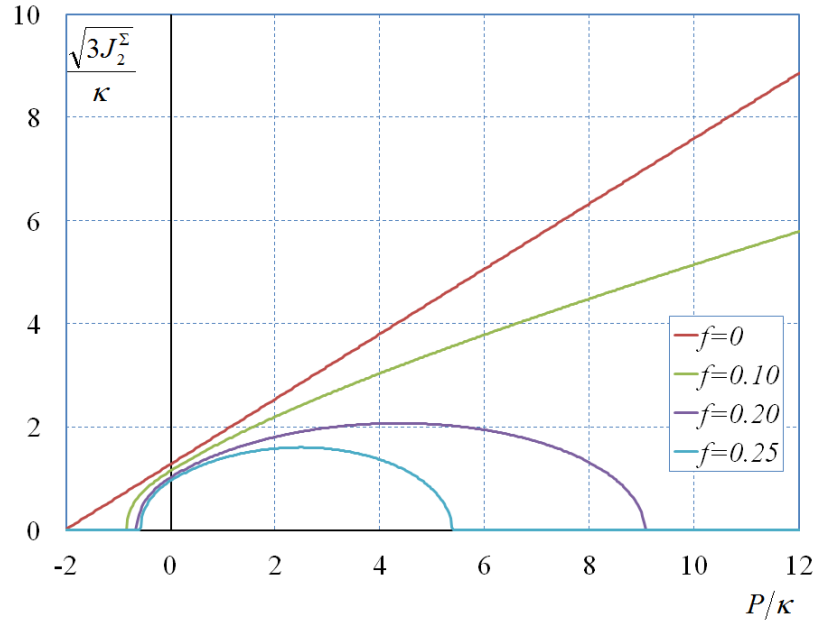


Figure 5: Yield criterion of Eq. (29) for the void-matrix aggregate plotted in the meridional plane for various values of void volume fraction f , a fixed Lode angle ($\theta = 0$), $\alpha = 0.164$, $\kappa = 1.648$ MPa, $\beta = 1.5$ and $\gamma = 0.95$.

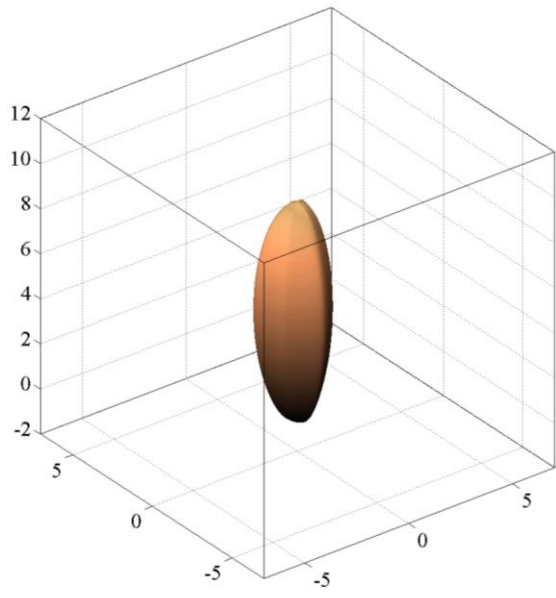


Figure 6: Yield criterion of Eq. (29) for the void-matrix aggregate plotted in 3D (rotated) principal stress space for a fixed value of damage ($f = 0.20$) with $\alpha = 0.164$, $\kappa = 1.648$ MPa, $\beta = 1.5$ and $\gamma = 0.95$.

SUMMARY AND CONCLUSIONS

Further investigation into the strength behavior of high explosives is necessary to understand and predict the sub-detonative response of energetic systems. This paper has focused on the derivation of a yield criterion to describe the pressure-dependent, strength-differential and damaged response of an energetic material. The approach utilized in deriving the

criterion is one that has been used heavily in the metal community—namely, the kinematic homogenization approach due to Hill and Mandel. The proposed criterion focused mainly on damage due to void growth. However, damage due to the cracking of energetic crystals is likely to dominate in many situations involving the loading of energetic materials. Damage due to cracking was only briefly discussed in this paper and the mechanism would need to be added to the proposed criterion through the addition of appropriate nucleation and evolution laws. Thus, the damage presented in this paper and its coupling with the material's strength should be considered as a general damage variable (since it needs to describe both damage due to void evolution and damage due to grain cracking), and not simply a porosity or void volume fraction.

While the proposed yield criterion captures some important features for the class of materials under investigation, some unanswered questions and challenges remain.

- The proposed yield criterion assumed a rigid, plastic response of the representative volume element, with all damage evolution occurring due to plastic flow. How accurate is this assumption for energetic materials (e.g., might there be significant visco-elastic effects in the aggregate response due to polymer binders)?
- Metallic models derived using homogenization techniques (e.g., Gurson) have significant issues accurately incorporating the strength response of the damage-free material into the response of the aggregate. It seems reasonable to expect that these same issues might exist for energetic materials as well.
- The proposed yield criterion assumed a spherical void embedded in a spherical RVE to develop its functional form. While some pre-existing voids exist in typical batches of high explosives, the void volume fraction tends to be fairly low (< 5 %). The more important damage mechanism, especially under compression, would seem to be the formation of new surfaces due to the shearing and cracking of the energetic crystals. How well can the proposed yield criterion handle the effects of such damage mechanisms if these effects are incorporated after-the-fact (e.g., in some damage nucleation and/or evolution law)?

Future work will need to incorporate damage due to the cracking of energetic crystals into the proposed yield criterion and implement the combined model into a finite element code. Once the model is implemented into some computational tool, the model's predictions can be compared with those from either experimental data or unit cell calculations (where voids and/or cracks are explicitly modeled). This model assessment should provide information concerning whether the simplifying assumptions made in developing the model are overly-restrictive.

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