

Thermodynamic Derivation of Yield Envelope Shapes

E.T.R. Dean¹

Summary

The shapes of yield envelopes for soils and other materials are generally taken as the starting point of a macroscopic plasticity model. This paper shows that these shapes can be accurately predicted using recent advances in thermodynamics and the new concept of multi-scale patterns. Some implications for future models are discussed.

keywords: Patterns, Thermodynamics, Yield Envelopes.

Introduction

Early proposals for the shape of a yield envelope include the Tresca envelope and the von Mises envelope (Efunfa, 2006). The latter can be related to the thermodynamic concept of energy. Hill (1950) described a theory of plasticity that started with an assumed yield envelope shape, and involved the idea of a flow rule. Roscoe, Schofield, and Wroth (1958) describe concepts of yielding of soils related to volumetric hardening, softening, and critical states. In Cam-Clay models for soil, the shape of a yield envelope is deduced from an assumed flow rule and the idea of associated flow.

In steel frame plasticity, a yield envelope for a structure is deduced in a disciplined way, from (a) the equilibrium and compatibility relations between structural elements, and (b) the material behaviours that occur at plastic hinges (eg Baker, Horne, and Heyman, 1965). This paper shows that published yield envelopes for soils can be deduced in an almost identical, disciplined way, by replacing plastic hinges with material elements that Dean (2005) called "patterns".

Patterns

In steel frame plasticity, a mechanism is a mode of collapse of a structure. The mechanism is formed as a result of the development of plastic hinges or other large strain features. Contrary to this, based on Loret's (1990) review, a "mechanism" in continuum plasticity is something which, together with other mechanisms, creates the elastic-plastic behaviour of a continuum. Other concepts of forming overall behaviour from elements include multilaminates (Pande and Sharma, 1983), multiple yield functions (Koiter, 1960), multiple substructures (Bucher et al, 2004), and others.

If we look at individual particles of sand, they have organization at many scales. Terzaghi, Peck, and Mesri (1996) present a series of micrographs of different sands. At low magnification, Ottawa sand particles look smooth, and the particles may be regarded as "bumps" with a size of about 1mm. We might believe that interparticle

¹University of the West Indies. Email: rdean@eng.uwi.tt.

contacts can be modeled as points. If we look at the surfaces of particles in contact, we see roughness – bumps that are an order of magnitude smaller. Perhaps inter-particle contacts are "points" of this size? But no, if we look at an individual bump at larger magnification, it too has a highly irregular surface. What this tells us is that, although we believe strongly that inter-particle contacts dominate the engineering behaviours of silica sands, the concepts of "contact", "size" and "roughness" can be applied at many different scales.

If we look at many particles of soil in a soil aggregate, we see order at various scales. Terzaghi, Peck, and Mesri (1996) describe how platy clay particles can aggregate together to form stacks, or loose structures with edge-to-edge contacts, or other structures. At larger scale, anisotropy in clays is sometimes attributed to the deposition of particles in preferential orientations. Dean (2005) proposed that the geometric arrangements of particles relative to one another would have order at many different scales, and that the important feature was not the scale, nor the type of order, but the fact that order would develop. He proposed that order would manifest itself as diffuse groupings of entities, such as groupings of particles, of stacks of particles, of collections of stacks, and so on. Groupings would interact with each other as well as with macroscopic stress and strain conditions imposed on the soil aggregate as a whole. He proposed to use the word "patterns" to indicate this.

A pattern might be defined as a collection of entities that act together in some partially coordinated or related way. An entire soil body might consist of a number of patterns. The entities might be subsets of the particles and voids of the body, or might be more abstract. Some particles and voids might be part of more than one pattern at any given time, and might be part of a different pattern at another time. The following sketch shows how a soil might appear if we shaded particles of one pattern grey, and drew outlines of the particles of the other patterns.

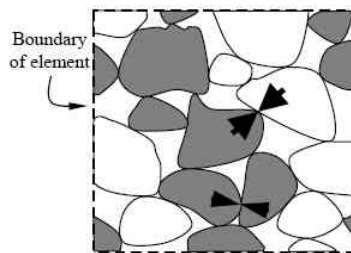


Figure 1: Particles and patterns. Big arrows are forces

Geometric properties of one pattern may be different to those of another pattern – eg, one pattern might be densely packed while another is loose. Effective stress in this sketch is something that crosses the boundary of the element. But there

are also forces between patterns, they are the forces between particles of the grey pattern and particles of other patterns. The idea of stress for a pattern will be a generalization of the idea of effective stress for the aggregate. And one pattern can do work on another during an incremental process.

The constitutive behaviour of the soil as a whole would be a result of the behaviours of patterns, modified by interactions between patterns, and by relations of compatibility and equilibrium. There is a correspondence between the idea of patterns and the idea of plastic hinges in a steel frame. But patterns are in contact with each other in a much more intimate way, at many different inter-particle contacts. Consequently, the mechanics of patterns will be somewhat more complex than that of steel frames.

Compatibility Equations for Patterns

In steel frame plasticity, compatibility equations relate the geometry of plastic hinges to the geometry of the steel frame. In the same way, compatibility equations can be proposed to relate the geometry of patterns to the geometry of a macroscopic soil element. We normally characterize the latter by strains. In the present paper we will consider only axial deformations, without principal axis rotations. Hence we need only consider principal strains e_1 , e_2 , and e_3 .

Probably the first geometric characteristic to consider would be specific volume. In order to explore the idea of compatibility for patterns, let us consider a simple relation between the specific volumes V_1 , V_2 , and V_3 of three soil patterns, and the strains of the soil as a whole:

$$\left. \begin{aligned} V_1 &= \alpha_1 \cdot V_o / \exp\{(1 - 2A) \cdot e_1 + A \cdot e_2 + A \cdot e_3\} \\ V_2 &= \alpha_2 \cdot V_o / \exp\{(1 - 2A) \cdot e_2 + A \cdot e_3 + A \cdot e_1\} \\ V_3 &= \alpha_3 \cdot V_o / \exp\{(1 - 2A) \cdot e_3 + A \cdot e_1 + A \cdot e_2\} \end{aligned} \right\} \quad (1)$$

where A is a material constant, V_o is the specific volume at some reference state, and α_1 , α_2 , α_3 are some internal, kinematic variables. Differentiating gives an incremental compatibility equation which can be written:

$$\begin{bmatrix} -dV_1/V_1 \\ -dV_2/V_2 \\ -dV_3/V_3 \end{bmatrix} = \begin{bmatrix} -d\alpha_1/\alpha_1 \\ -d\alpha_2/\alpha_2 \\ -d\alpha_3/\alpha_3 \end{bmatrix} + \begin{bmatrix} dv_{1u} \\ dv_{2u} \\ dv_{3u} \end{bmatrix} \quad (2a)$$

$$\text{with: } \begin{bmatrix} dv_{1u} \\ dv_{2u} \\ dv_{3u} \end{bmatrix} = \begin{bmatrix} 1 - 2A & A & A \\ A & 1 - 2A & A \\ A & A & 1 - 2A \end{bmatrix} \cdot \begin{bmatrix} de_1 \\ de_2 \\ de_3 \end{bmatrix} \quad (2b)$$

The quantities $dv_{i,u}$ are determined by the imposed strain increments, and might be interpreted as externally-imposed volume strains of the three patterns. The param-

eter A is a cross-coupling term. It ensures that each pattern feels effects from all principal strain directions.

Equilibrium Equations for Patterns

Peric, Owen, and Honnor (1990) describe application of the principle of virtual work or "work-conjuacy" to materials. Let $P_1^/$, $P_2^/$, and $P_3^/$ be scalar measures of effective stresses for patterns 1, 2, and 3 respectively. Let us suppose that, in any increment of behaviour, the incremental work dW done on the soil per unit volume of particles can be expressed as:

$$dW = dW_{1u} + dW_{2u} + dW_{3u} \quad (3a)$$

$$\text{with: } dW_{iu} = P_i^/ \cdot V_i \cdot dv_{iu} \quad (3b)$$

We might interpret dW_{iu} as "external work" for the i^{th} pattern. We can also express the work as:

$$dW = \sigma_1^/ \cdot V \cdot de_1 + \sigma_2^/ \cdot V \cdot de_2 + \sigma_3^/ \cdot V \cdot de_3 \quad (4)$$

where $\sigma_i^/$ are the principal effective stresses, and V is the specific volume of the material as a whole (Schofield and Wroth, 1968; Houlsby, 1979). Using (2) to substitute for the increments in (3), equating the result to (4), and imposing the condition that the equality applies for all possible independent increments de_i , gives:

$$\begin{bmatrix} \sigma_1^/ \\ \sigma_2^/ \\ \sigma_3^/ \end{bmatrix} = \frac{1}{V} \begin{bmatrix} 1-2A & A & A \\ A & 1-2A & A \\ A & A & 1-2A \end{bmatrix} \begin{bmatrix} P_1^/ \cdot V_1 \\ P_2^/ \cdot V_2 \\ P_3^/ \cdot V_3 \end{bmatrix} \quad (5)$$

This equation may be interpreted as an equilibrium relation between pattern stresses and externally imposed stresses. Its derivation was analogous to the derivation of equilibrium equations in steel frame plasticity. The inverse exists if A is not 1, and is such that:

$$P_i^/ V_i = \frac{1}{3} \cdot \frac{(\sigma_i^/ - A \cdot p^/) \cdot V}{1 - A} \quad (6)$$

where $p^/$ is the average of the 3 principal effective stresses.

For some calculations in this paper, it will be useful to consider conditions in the triaxial cell, shown below.

The radial effective stresses are equal. The triaxial deviator stress q is the difference between the axial and radial stresses, being positive if the axial stress is greater (Schofield and Wroth, 1968; Wood, 1984).

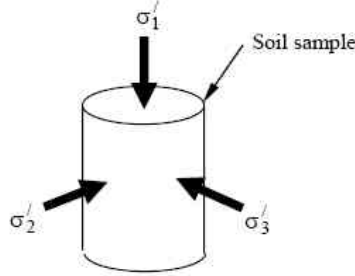


Figure 2: Effective soil stresses in triaxial test ($\sigma_2' = \sigma_3'$)

Energy properties of patterns

Since patterns contain particles, and particles are physical objects that obey laws of thermodynamics, it follows that patterns will have aggregate thermodynamic properties like internal energy, free energy, entropy. Of particular interest here is Helmholtz free energy, described by Collins and Houlsby (1997), Houlsby and Puzrin (2000), and others. Let us suppose, for the purpose of exploring this idea, that the Helmholtz free energy F_i of the i^{th} pattern is given by:

$$F_i = \frac{\kappa}{1 - \kappa} \mu_i \cdot P_i' \cdot V_i \quad (7)$$

where κ is a material constant in the range 0 to 1, and μ_i is a kinematic variable which we might call the memory of the i^{th} pattern. We shall not be much concerned about memory in this paper, and will generally assume that its value is 1, but it is good to have the ability to explore memory effects at some future date.

The Helmholtz free energy involves a component due to internal energy and a component associated with entropy. We might naturally expect both of these components to be limited in some way. Let us suppose, for the purpose of exploring this idea, that the limiting Helmholtz free energy of a pattern, denoted herein as $F_{asy,i}$, is directly related to the pattern's specific volume V_i , by:

$$F_{asy,i} = \frac{\kappa}{1 - \kappa} \frac{\exp(\Gamma/\lambda)}{(V_i)^{(1-\lambda)/\lambda}} \quad (8)$$

where Γ and λ are material constants and λ is in the range κ to 1. Experimental data of proportional straining processes, such as data by Topolnicki, Gudehus, and Mazurkiewicz (1990) for clays, and Chu and Lo (1993) for sands, indicate that most limits in soils are approached asymptotically. It is good to use the subscript *asy*, because it will let us extend our theory later to asymptotic processes.

There will be some soil states at which the i^{th} pattern's Helmholtz free energy equals its limit. Putting $F_i = F_{asy,i}$ and simplifying the result gives:

$$\ln(V_i) + \lambda \cdot \ln(P_i') = \Gamma - \lambda \cdot \ln(\mu_i) \quad (9)$$

Figure 3 shows this as a line in a stress-volume space for the i^{th} pattern.

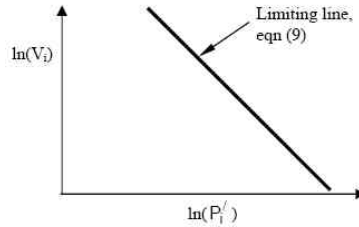


Figure 3: Stress-volume space for the i^{th} pattern

Let us consider only the case $\mu_i=1$. Then all states below and to the left of this line have Helmholtz free energies that are less than the limit, and all states to the right have Helmholtz free energies that are greater than the limit. Hence we might guess that the limiting line has something to do with yielding. Perhaps states to the left and below the line are elastic, and the line itself represents a yield envelope for a pattern? Let us check. Consider the special, isotropic case when the soil has simply been compressed isotropically, so that each principal effective stress equals p' , and $q=0$. If all patterns are in identical states and the kinematic variables α_i in (1) are all 1, then (1) implies that the pattern specific volumes all equal the overall specific volume V , and (6) implies that the pattern stresses all equal one third of the mean normal effective stress p' . Substituting in (9) gives:

$$\ln(V) + \lambda \cdot \ln(p') = \Gamma - \lambda \cdot \ln(\mu_i/3) \quad (10)$$

If $\mu_i = 1$, the right side is a constant, and the equation may be interpreted as the Butterfield (1979) version of the virgin isotropic compression line. States to the left and below this line in (p', V) space are more or less elastic, and yielding occurs when the soil state reaches the line.

We have thus discovered that the familiar virgin isotropic compression line for soils can be interpreted as a consequence of the thermodynamics of patterns.

Incremental work equations

Examination of Figure 1 shows that there are inter-particle forces in which the particles involved are from different patterns. Therefore, when these contacts displace in an incremental process, one pattern will do work on another pattern, with magnitude equal to the force times the displacement. There may also be some slip. We could adopt a strategy that the work done in slip is assigned in some way to one or other of the patterns, or shared by both.

Based on these considerations, it seems appropriate to define the incremental work dW_i done on the i^{th} pattern as the sum of the incremental external work dW_{iu} calculated earlier, and the incremental work dE_i that is done on the i^{th} pattern by

other patterns:

$$dW_i = dW_{iu} + dE_i \quad (11)$$

If we ensure that dissipation at these particle contacts is appropriately assigned to patterns, then the remaining work is such that, at any contact, the work done by one pattern on a second equals the work done by the second on the first. Hence the sum of energy transfers dE_i for all patterns is zero, and the sum of the pattern works dW_i equals the net work dW done on the soil.

Collins and Houlsby (1997) showed that, for the material as a whole, the rate of working is the sum of a rate of change of Helmholtz free energy, and a strictly non-negative rate of dissipative work. In incremental form, we can propose that work dW_i done on the i^{th} pattern is the sum of the increment dF_i of the pattern's Helmholtz free energy and a strictly non-negative increment $dW_{i,d}$ which we might call the dissipation in the pattern:

$$dW_i = dF_i + dW_{i,d} \quad (12)$$

dF_i is not in general the same as incremental elastic work, because it may include work due to change of memory, which might not necessarily be elastic. Hence $dW_{i,d}$ is not in general the same as plastic work. The above equation is subtly different from the familiar separation of work into elastic and plastic components.

Yield envelopes – derivation of equations

Let us guess that a yield envelope in effective stress space is associated with a combination of the limiting lines (9) for all three patterns. There will be some point A on the envelope where all patterns are on their respective limiting lines. There may be other points where only two of the patterns are at their limits, with the third pattern below its limit. There may be points where only one pattern is at its limit.

Consider point A in principal effective stress space. Let us suppose that the sample is unloaded from A, and then reloaded along a different path, reaching yield at point B. For simplicity we make the following assumptions:

- (a) the unload reload path is elastic from A to B
- (b) incremental energy transfers dE_i occur only in association with dissipation, so $dE_i=0$ all along AB
- (c) changes of memory in this process are negligible
- (d) the energy limits $F_{asy,i}$ evolve along the elastic path only in association with overall volume strain; details below

From assumptions (a) and (b), together with (11) and (12), we deduce that in any increment along AB, the change of energy dF_i for the i^{th} pattern equals the external work done on that pattern. Hence using (2), (3), and (7):

$$\frac{dF_i}{F_i/\mu_i} = \frac{1-\kappa}{\kappa}((3-2A).d\varepsilon_i + A.d\varepsilon_{i+1} + A.d\varepsilon_{i+2}) \quad (13)$$

where subscripts $i+1$ and $i+2$ cycle through 1,2,3 (so, if $i=2$, then $i+1=3$, but if $i=3$, then $i+1=1$). By assumption (c), μ_i is practically constant, so we can add the equations for all three patterns and integrate along path AB, giving:

$$\left(\frac{F_{1,B}}{F_{1,A}}\right)^{\mu_1} \cdot \left(\frac{F_{2,B}}{F_{2,A}}\right)^{\mu_2} \cdot \left(\frac{F_{3,B}}{F_{3,A}}\right)^{\mu_3} = \left(\frac{V_A}{V_B}\right)^{3(1-\kappa)/\kappa} \quad (14)$$

where subscripts A and B refer to states A and B respectively, and the ratio of specific volumes on the right occurs because incremental volume strain $-dV/V$ equals the sum of the principal strains $d\varepsilon_i$. Differentiating (8) gives:

$$\frac{dF_{asy,i}}{F_{asy,i}} = -\frac{1-\lambda}{\lambda} \cdot \frac{dV_i}{V_i} \quad (15)$$

We might say that the i^{th} pattern "hardens" if its energy limit increases, and softens if it decreases. In (2), the incremental specific volumes are related not only to external strain increments, but also to the kinematic increments $d\alpha_i$. Consequently, (15) is unlikely to be usable as a hardening equation – it is more likely to be an evolution law for the specific volumes V_i . We may thus expect that there will be a separate hardening law which will determine $dF_{asy,i}$. Let us guess that this separate law will involve effects of volume strains, plasticity and dissipation, and perhaps shear strains also. Let us suppose that the major effect is due to volume strain. Then we might guess that, for the path AB that we are considering, the energy limits evolve according to an equation similar to (15), but with V_i replaced by the overall specific volume V . Integrating then gives:

$$\frac{F_{asy,i,B}}{F_{asy,i,A}} \approx \left(\frac{V_A}{V_B}\right)^{(1-\lambda)/\lambda} \quad (16)$$

where the approximately equals sign is used because we may have omitted some effects. Suppose point B in stress space represents an event in which the i^{th} pattern reaches its limiting line in its stress-volume space. Then $F_{i,B}$ in (15) equals $F_{asy,i,B}$ in (16). Using this equality, together with (6) and (7), and eliminating the volume ratio V_A/V_B , gives:

$$\left(\frac{\sigma'_{1B} - Ap'_{1B}}{\sigma'_{1A} - Ap'_{1A}}\right)^{\mu_1} \left(\frac{\sigma'_{2B} - Ap'_{2B}}{\sigma'_{2A} - Ap'_{2A}}\right)^{\mu_2} \left(\frac{\sigma'_{3B} - Ap'_{3B}}{\sigma'_{3A} - Ap'_{3A}}\right)^{\mu_3} \approx \left(\frac{\sigma'_{iB} - Ap'_{iB}}{\sigma'_{iA} - Ap'_{iA}}\right)^n \quad (17a)$$

$$\text{with: } n = 3 \frac{\lambda}{\kappa} + \lambda \cdot \sum_{j=1}^3 (\mu_j - 1) \tag{17b}$$

Point B in the i^{th} pattern’s stress-volume space would be a state at which that pattern would be begin to yield plastically. In effective stress space, the collection of points specified by the above equation form a surface that passes through point A. The surface might be interpreted as the yield surface that is associated with yield in the i^{th} pattern. By combining three such equations together, one for each of the three patterns $i=1, 2,$ and $3,$ we get three surfaces which together will form a yield envelope in stress space.

Yield envelopes – comparisons with published data

Figure 4 shows a comparison of a calculated yield envelope with experimental data of yield points by Tavenas and Leroueil (1977, 1978) for St Alban clay. The clay has low to medium plasticity. Samples were from depths of 3 to 6 metres, with vertical pre-consolidation pressures of 51 to 92 kPa, and over-consolidation ratios around 2. The data were read from Figure 20.5 of Terzaghi, Peck, and Mesri (1996), then converted to the Cambridge parameters (p',q) (Wood, 1984). Normalized parameters are used in Figure 4. All the memories were taken as 1. The theory matches the data well.

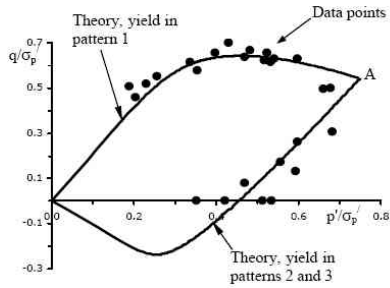


Figure 4: Theory and experiment – St.Alban Clay

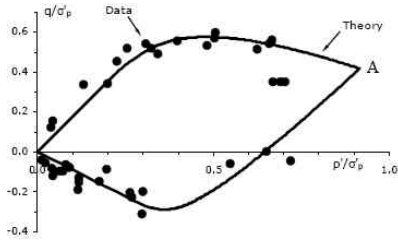


Figure 6: Theory and experiment – Drammen Clay

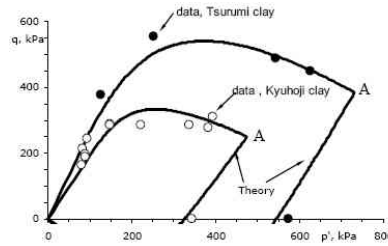


Figure 5: Theory and experiment – Osaka Bay Clays

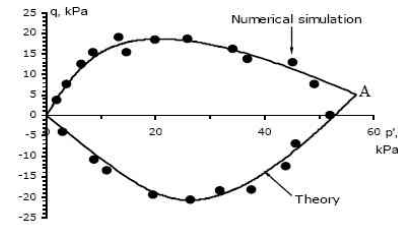


Figure 7: Theory and computer – Crushable conglomerates

Figure 5 shows comparisons for two Pleistocene marine clays from Osaka Bay, Japan. Data were read from Figure 5 of Yashima et al (1999). The clays are well-structured, natural clays, with relatively high natural water contents due to diatoms. The theory matches the data well.

Figure 6 shows a comparison for yield points by Larrson (1980) and Larrson and Sallfors (1981) for Drammen clay. Again, the memories were assumed equal to 1. The data were read and re-plotted from Figure 20.6 of Terzaghi, Peck, and Mesri (1996). The theory matches the data fairly well.

Figure 7 shows a comparison of model calculations with results for numerical simulations of crushable conglomerates by Cheng et al (2004). The data were read and re-plotted from Cheng et al's Figure 3. The memories were assumed to be 1. The model matches the simulations well.

Discussion and Conclusions

This paper has shown that, by combining the mechanical concept of patterns with recent advances in thermodynamics, one can accurately predict and explain the familiar isotropic virgin compression line for soils, and yield envelope shapes for natural clays and for numerical assemblies of particles.

The theoretical development was highly disciplined, using compatibility, equilibrium, and material behavior in a way that is analogous to the theory of steel frame plasticity. No assumptions have been made about the nature of patterns or the scale at which they have effects, and only very global assumptions are involved in the general work equations (11) and (12). One may therefore expect this theory to be applicable to a wide variety of materials, scales, and geometries. For example, yield envelopes for foundations as a whole are discussed by Bienen, Byrne, Houlsby, and Cassidy (2006) and others. This new theory can be used to deduce yield envelopes in force-resultant space for footings.

The theory as presented in this short paper is incomplete in the sense that a detailed hardening law has not been specified. Evolutions of the kinematic variables α_i and memory variables μ_i are not addressed herein. The theory here is also specialized in the sense that particular equations have been used to explore ideas. Different forms for the compatibility equation (1), for example, would lead to different equations for yield envelopes.

Ongoing developments show that the same fundamental ideas provide new rules for realistic modeling of monotonic and cyclic stress-strain behaviors. The future looks bright for this new theory.

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