An approach to plasticity based on generalised thermodynamics

G.T. HOULSBY[1] and A.M. PUZRIN[2]

[1] University of Oxford, UK
[2] Technion-Israel Institute of Technology, Israel

Abstract. The starting point for this paper is the problems encountered in conventional plasticity when the thermodynamics of plastic materials is considered. These problems provide the motivation for an alternative formulation, based on thermomechanical principles. In this formulation, a constitutive model is defined solely by specification of two thermodynamic potentials: an energy function and a dissipation function (or a yield function). Incremental response of the material is derived from these scalar potential functions using standard procedures. Next, a simple classification of constitutive models is introduced, based on the form of their potential functions. Further generalisation of this framework allows some important issues in modern plasticity theory to be addressed. Finally, some directions for future developments are proposed.

1 Introduction

In this paper we describe an approach to constitutive modeling based on generalized thermodynamics. This work has its roots principally in the work of Ziegler (1977, 1983), as developed for plasticity theory by Houlsby (1981, 1982, 1996) and Collins & Houlsby (1997). It also has much in common with the work of Maugin (1992) and Coussey (1995). Further extension and generalisation of this approach was made by Houlsby & Puzrin (1999) and Puzrin & Houlsby (1999). For more detailed mathematical derivations a reader should refer to these papers.

In conventional plasticity, derivation of incremental response requires specification of the following:

- a relationship for the elastic component of strain;
- a yield surface;
- the flow rule or plastic potential;
- a hardening rule, including strain hardening and yield surface translation rules.

How do the First and Second Laws of Thermodynamics feature within the theory? In conventional plasticity they are not a part of formulation. In the best cases, some quasi-thermodynamic principles are applied *post hoc*. The best example of the latter approach is Drucker's Stability Postulate. Subject to some conditions, materials which satisfy the postulate are thought also to satisfy the Second Law of Thermodynamics, but the postulate itself it is not a Law, and is known to be a classification only. It imposes convexity of the yield surface and normality of incremental plastic strain vector to the yield surface, *i.e.* an associated flow. However, the normality assumption is violated by many geomaterials exhibiting frictional behaviour. Many counter examples to Drucker's Postulate are known, both in the form of conceptual models and from experimental data.

Clearly, there is a need for an alternative formalism, which should allow for the following objectives to be achieved:

- the Laws of Thermodynamics should be obeyed for all models, even those with non-associated flow;
- a compact and consistent framework should be created for constitutive modeling;
- models should be able to be compared, and new models developed easily within a single framework;
- more general Uniqueness and Bound Theorems should be derived for materials with non-associated flow.

2 Thermomechanical formulation

The alternative formalism proposed here is based on direct use of thermodynamic potentials (Figure 1). Incremental response is derived from two scalar potential functions: an energy function and a dissipation function (or yield function). The energy function can be used in any of four alternative forms related by Legendre transformations. An alternative to the dissipation function is a yield surface, related to the dissipation function by a degenerate Legendre transformation.

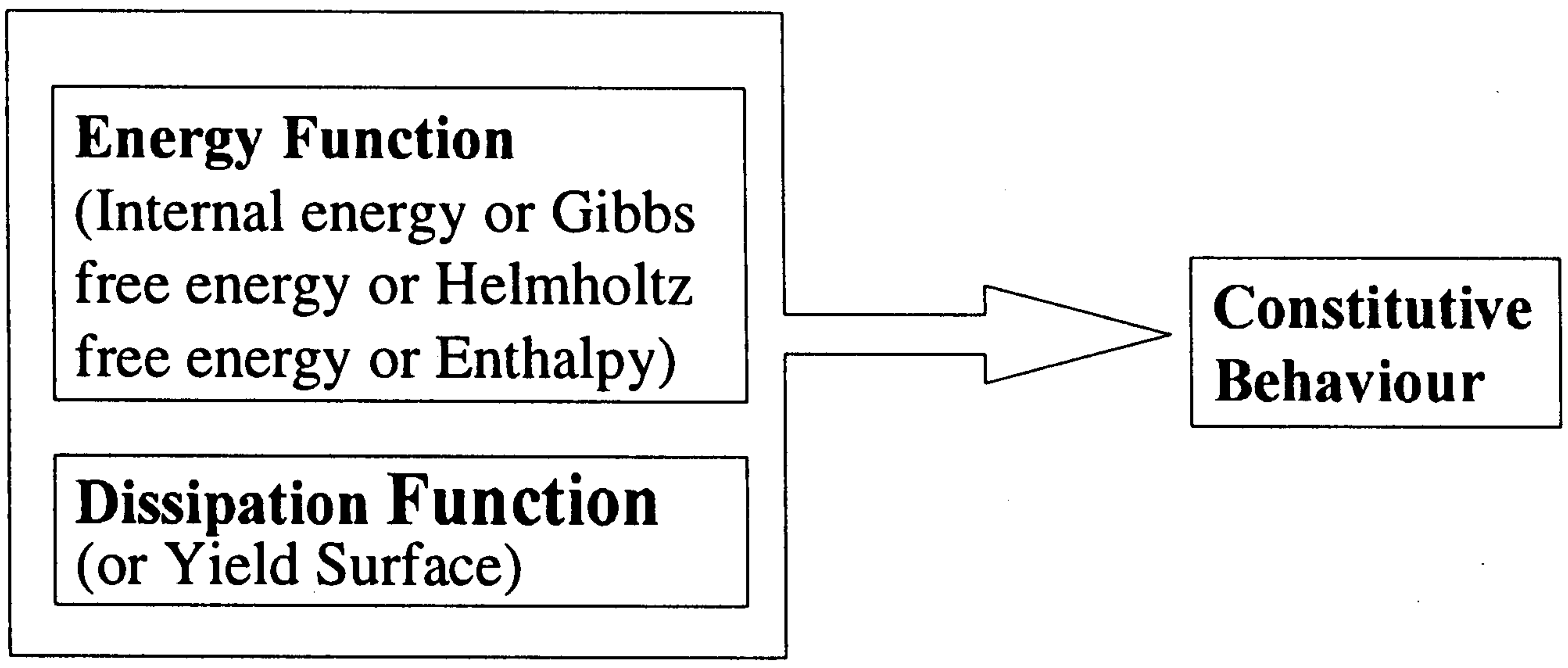


Fig. 1. Schematic layout of the thermomechanical framework

2.1 Energy Function

We start with an energy function. Energy functions for small strain continuum mechanics in Cartesian coordinates are defined in table 1: u is the specific internal energy function of strain tensor $\varepsilon_{\mathrm{ij}}$ and specific entropy s, defined as a potential for stress tensor σ_{ij} and temperature θ. The function f is the specific Helmholtz free energy function of strain tensor and temperature, a potential for stress and specific entropy; h is the specific enthalpy function of stress and temperature, a potential for strain and entropy; and finally g is the specific Gibbs free energy function of stress and entropy, a potential for strain and temperature.

Internal energy	**Helmholtz free energy**	**Enthalpy**	**Gibbs free energy**
$u=u(\varepsilon_{ij},s)$	$f=f(\varepsilon_{ij},\theta)$	$h=h(\sigma_{ij},s)$	$g=g(\sigma_{ij},\theta)$
$\sigma_{ij}=\dfrac{\partial u}{\partial \varepsilon_{ij}}$ $\theta=\dfrac{\partial u}{\partial s}$	$\sigma_{ij}=\dfrac{\partial f}{\partial \varepsilon_{ij}}$ $s=-\dfrac{\partial f}{\partial \theta}$	$\varepsilon_{ij}=-\dfrac{\partial h}{\partial \sigma_{ij}}$ $\theta=\dfrac{\partial h}{\partial s}$	$\varepsilon_{ij}=-\dfrac{\partial g}{\partial \sigma_{ij}}$ $s=-\dfrac{\partial g}{\partial \theta}$
$u=g-s\theta-\sigma_{ij}\varepsilon_{ij}$	$f=u-s\theta$	$h=u-\sigma_{ij}\varepsilon_{ij}$	$g=h-s\theta$ $=f-\sigma_{ij}\varepsilon_{ij}$

Table 1. Energy function for small strain continuum mechanics.

These functions differ slightly from those used in the thermodynamics of fluids, mainly in that they are defined per unit volume, not per unit mass. The functions are not independent: given any one of them, the other three are obtained by partial or complete Legendre transformations. To get a general impression of these functions, consider the following example, corresponding to the case of isotropic thermoelasticity:

$$u=\frac{3K}{X}\frac{\varepsilon_{ii}\varepsilon_{jj}}{6}+2G\frac{\varepsilon'_{ij}\varepsilon'_{ij}}{2}-\frac{\alpha 3K\theta_0}{cX}s\varepsilon_{kk}+\frac{\theta_0}{cX}\frac{s^2}{2}+s\theta_0, \tag{1a}$$

$$f=3K\frac{\varepsilon_{ii}\varepsilon_{jj}}{6}+2G\frac{\varepsilon'_{ij}\varepsilon'_{ij}}{2}-\alpha 3K\left(\theta-\theta_0\right)\varepsilon_{kk}-\frac{cX}{\theta_0}\frac{\left(\theta-\theta_0\right)^2}{2}, \tag{1b}$$

$$h=-\frac{X}{3K}\frac{\sigma_{ii}\sigma_{jj}}{6}-\frac{1}{2G}\frac{\sigma'_{ij}\sigma'_{ij}}{2}-\frac{\alpha\theta_0}{c}s\sigma_{kk}+\frac{\theta_0}{c}\frac{s^2}{2}+s\theta_0, \tag{1c}$$

$$g=-\frac{1}{3K}\frac{\sigma_{ii}\sigma_{jj}}{6}-\frac{1}{2G}\frac{\sigma'_{ij}\sigma'_{ij}}{2}-\alpha\left(\theta-\theta_0\right)\sigma_{kk}-\frac{c}{\theta_0}\frac{\left(\theta-\theta_0\right)^2}{2}. \tag{1d}$$

Where K is the isothermal bulk modulus, G the shear modulus, α the coefficient of thermal expansion, c the specific heat at constant stress, θ the initial temperature and $X = 1 - \left(9K\alpha^2\theta_0/c\right)$. The other variables are conventional stress and strain tensors, temperature and specific entropy. A prime notation is used for deviatoric components of stress and strain tensors.

2.2 Dissipation Function

The second potential function required in the thermomechanical formulation is the dissipation function, which allows the Second Law of Thermodynamics to be satisfied within the proposed framework. The Second Law can be formulated as the following inequality, where the term in brackets is the entropy flux:

$$\dot{s} \geq -\left(\frac{q_k}{\theta}\right)_{,k} \tag{2}$$

When this inequality is rewritten in the following way:

$$\theta\dot{s} + q_{k,k} - \frac{q_k\theta_{,k}}{\theta} \geq 0 \tag{3}$$

the first two terms $\theta\dot{s} + q_{k,k} = d$ are called the mechanical dissipation. The third term is called the thermal dissipation and it is always non-negative. For slow processes, this term becomes small by comparison with the first two, so it is argued that the mechanical dissipation must itself be non-negative. This requirement is a slightly more stringent condition than the Second Law, but is widely accepted.

So far we defined the mechanical dissipation, but what about the dissipation function? For dissipative materials, the internal energy is a function not only of strain and entropy, but of kinematic internal variables α_{ij} as well: $u = u\left(\varepsilon_{ij}, \alpha_{ij}, s\right)$. Strain, entropy and internal variables define a thermodynamic state of material. We then make an assumption that the dissipation is also a function of the thermodynamic state of the material. Moreover, it is not only a function of state, but also of the rate of change of this state. In fact we shall consider only those mechanisms where dissipation depends only on one rate - the rate of change of the internal variable: $d = d^u\left(\varepsilon_{ij}, \alpha_{ij}, s, \dot{\alpha}_{ij}\right) \geq 0$. Note, that the corresponding dissipation function can be defined for each of the four energy functions, and that it should be non-negative to satisfy the Second Law of Thermodynamics.

2.3 Ziegler's Orthogonality Condition

Next, we need to impose the First Law of Thermodynamics, but first let us define the generalised and dissipative generalised stress tensors. The generalised stress tensor is defined by differentiation of an energy function with respect to internal variable:

$$\bar{\chi}_{ij} = -\frac{\partial u}{\partial \alpha_{ij}} = -\frac{\partial f}{\partial \alpha_{ij}} = -\frac{\partial h}{\partial \alpha_{ij}} = -\frac{\partial g}{\partial \alpha_{ij}} \tag{4}$$

The dissipative generalised stress tensor is defined by differentiation of a dissipation function with respect to internal variable rate:

$$\chi_{ij} = \frac{\partial d^e}{\partial \dot{\alpha}_{ij}} \tag{5}$$

where e stands for any of u, f, h or g.

The First Law of Thermodynamics states that rate of change of internal energy is the sum of the mechanical power and the rate of heat supply to an element of volume:

$$\dot{u} = \sigma_{ij}\dot{\varepsilon}_{ij} - q_{k,k} = \sigma_{ij}\dot{\varepsilon}_{ij} + \theta\dot{s} - d \tag{6}$$

On the other hand, the internal energy rate can be defined by the fact that internal energy is a function of state:

$$\dot{u} = \frac{\partial u}{\partial \varepsilon_{ij}}\dot{\varepsilon}_{ij} + \frac{\partial u}{\partial \alpha_{ij}}\dot{\alpha}_{ij} + \frac{\partial u}{\partial s}\dot{s} \tag{7}$$

Comparing expressions (6) and (7), and using the fact that internal energy function is a potential for stress and temperature, we conclude that the third terms are equal. Then, using the definition of the generalised stress (4), we obtain an expression for mechanical dissipation:

$$d = \bar{\chi}_{ij}\dot{\alpha}_{ij} \tag{8}$$

A similar expression for dissipation, but this time through the dissipative generalised stress, can be obtained if we limit our analysis to rate-independent materials. In rate-independent materials, dissipation function has to be homogeneous of order one in the rates of the internal variable, because there is no characteristic time. In this case, using Euler's theorem and definition of the dissipative generalised stress (5) we obtain an alternative expression for the dissipation function:

$$d = \frac{\partial d^e}{\partial \dot{\alpha}_{ij}}\dot{\alpha}_{ij} = \chi_{ij}\dot{\alpha}_{ij} \tag{9}$$

At first sight, expressions (8) and (9) imply equality between the generalised and dissipative generalised stress tensors. In fact, we can draw only much weaker conclusion that their difference is always orthogonal to internal variable rate vector: $(\bar{\chi}_{ij} - \chi_{ij})\,\dot{\alpha}_{ij} = 0$. Ziegler (1977) argues, however, that a stronger statement of equality can be made:

$$\bar{\chi}_{ij} = \chi_{ij} \tag{10}$$

This assumption is termed Ziegler's Orthogonality Condition. Without entering the debate about whether this assumption is valid, we follow Ziegler's approach here, using it simply to investigate a subset of models in a hope that it will include models with non-associated flow.

2.4 A bridge to conventional plasticity

At his stage the thermomechanical formulation is complete, but in order to link it to conventional plasticity we need some additional elaboration. We have already used the fact that for rate-independent materials, the dissipation function is homogeneous of order one in internal variable rates. In this case, we can define a yield function as a degenerate special case of the Legendre transformation of the dissipation function: $y^e = \chi_{ij}\dot{\alpha}_{ij} - d^e = 0$, where $y = y^u(\varepsilon_{ij}, \alpha_{ij}, s, \chi_{ij}) = 0$, $y = y^f(\varepsilon_{ij}, \alpha_{ij}, \theta, \chi_{ij}) = 0$, $y = y^h(\sigma_{ij}, \alpha_{ij}, s, \chi_{ij}) = 0$ or $y = y^g(\sigma_{ij}, \alpha_{ij}, \theta, \chi_{ij}) = 0$. In practice, the yield function is derived in generalised stress space by eliminating internal variable rates from the equations for dissipative generalised stresses (5).

The flow rule follows from the properties of the Legendre transformation:

$$\dot{\alpha}_{ij} = \lambda \frac{\partial y^e}{\partial \chi_{ij}} \tag{11}$$

To find an analogy between this flow rule and the one utilized in conventional plasticity we need to assign a physical meaning to internal variables. It can be shown (Collins & Houlsby 1997), that for materials exhibiting no elastic-plastic coupling, the internal variable can be identified with the conventionally defined plastic strain. Then, we have a flow rule (11) linking the plastic strain rates to the derivatives of the yield surface but with respect to the generalised stresses, not to stresses as would be expected in conventional associated plasticity. This difference allows for some forms of a non-associated flow to be accommodated within this framework.

Finally we address the convexity of the yield function. From the condition that the dissipation function is non-negative, and from equations (9) and (11) it follows that the yield surface should contain the origin in generalised stress space and satisfy certain weak convexity conditions: $\chi_{ij} \frac{\partial y^e}{\partial \chi_{ij}} \geq 0$ (since $\lambda \geq 0$). It is not required, however, that the yield surface should be strictly convex either in generalised stress space or in stress space.

2.5 Summary

To summarize the development so far, the thermomechanical framework for rate-independent materials is based on the two fundamental hypotheses. The first is that the dissipation function is non-negative, which is a more stringent condition than the Second Law of Thermodynamics. The second is the Ziegler's Orthogonality Condition, which is more stringent than the First Law of Thermodynamics. In spite of that, the framework obtained is more flexible than that restricted by the Drucker's Stability Postulate, because:

- it does not require associated flow in true stress space;
- it does not require strict convexity in neither of stress spaces.

Returning to the original objectives, we are now able to obey the Laws of Thermodynamics for some classes of models with non-associated flow.

Within the proposed framework, two thermodynamic potentials define the entire constitutive behaviour. The first is an energy potential, while the second is either a dissipation function or the yield surface. However, there are 16 different possibilities for the choice of the potentials, representing all permutations on the following possibilities (Table 2):

- choice of one of the four energy functions;
- dissipation function or yield surface;
- transformation between the internal variable and the generalised stress for the energy function.

Energy function		u or $\bar{u}$	f or $\bar{f}$	h or $\bar{h}$	g or $\bar{g}$
Dissipation function $d^e \geq 0$	α_{ij}	$u(\varepsilon_{ij},\alpha_{ij},s)$ $d^u(\varepsilon_{ij},\alpha_{ij},s,\dot{\alpha}_{ij})$	$f(\varepsilon_{ij},\alpha_{ij},\theta)$ $d^f(\varepsilon_{ij},\alpha_{ij},\theta,\dot{\alpha}_{ij})$	$h(\sigma_{ij},\alpha_{ij},s)$ $d^h(\sigma_{ij},\alpha_{ij},s,\dot{\alpha}_{ij})$	$g(\sigma_{ij},\alpha_{ij},\theta)$ $d^g(\sigma_{ij},\alpha_{ij},\theta,\dot{\alpha}_{ij})$
	$\bar{\chi}_{ij}$	$^{-}(\varepsilon_{ij},\bar{\chi}_{ij},\ )$ $d^{\bar{u}}(\varepsilon_{ij},\bar{\chi}_{ij},s,\dot{\alpha}_{ij})$	$\bar{f}(\varepsilon_{ij},\bar{\chi}_{ij},\theta)$ $d^{\bar{f}}(\varepsilon_{ij},\bar{\chi}_{ij},\theta,\dot{\alpha}_{ij})$	$\bar{h}(\sigma_{ij},\bar{\chi}_{ij},s)$ $d^{\bar{h}}(\sigma_{ij},\bar{\chi}_{ij},s,\dot{\alpha}_{ij})$	$\bar{g}(\sigma_{ij},\bar{\chi}_{ij},\theta)$ $d^{\bar{g}}(\sigma_{ij},\bar{\chi}_{ij},\theta,\dot{\alpha}_{ij})$
Yield surface $y^e = 0$	α_{ij}	$u(\varepsilon_{ij},\alpha_{ij},s)$ $y^u(\varepsilon_{ij},\alpha_{ij},s,\chi_{ij})$	$f(\varepsilon_{ij},\alpha_{ij},\theta)$ $y^f(\varepsilon_{ij},\alpha_{ij},\theta,\chi_{ij})$	$h(\sigma_{ij},\alpha_{ij},s)$ $y^h(\sigma_{ij},\alpha_{ij},s,\chi_{ij})$	$g(\sigma_{ij},\alpha_{ij},\theta)$ $y^g(\sigma_{ij},\alpha_{ij},\theta,\chi_{ij})$
	$\bar{\chi}_{ij}$	$\bar{u}(\varepsilon_{ij},\bar{\chi}_{ij},s)$ $y^{\bar{u}}(\varepsilon_{ij},\bar{\chi}_{ij},s,\chi_{ij})$	$\bar{f}(\varepsilon_{ij},\bar{\chi}_{ij},\theta)$ $y^{\bar{f}}(\varepsilon_{ij},\bar{\chi}_{ij},\theta,\chi_{ij})$	$\bar{h}(\sigma_{ij},\bar{\chi}_{ij},s)$ $y^{\bar{h}}(\sigma_{ij},\bar{\chi}_{ij},s,\chi_{ij})$	$\bar{g}(\sigma_{ij},\bar{\chi}_{ij},\theta)$ $y^{\bar{g}}(\sigma_{ij},\bar{\chi}_{ij},\theta,\chi_{ij})$

Table 2. Energy function for small strain continuum mechanics.

In principle any of the 16 formulations could be used. However, currently, only four of them (the third row of Table 2) have been found to be convenient for derivation of incremental stress strain response.

2.6 Incremental stress-strain response

The finite element analysis of problems with nonlinear materials, usually requires the incremental form of the constitutive relationship. In the thermomechanical framework, the incremental response can be derived for each of the four energy formulations. The choice of a particular formulation depends on which variables are controlled: stress, strain, temperature or entropy. Then, the unknown variables are defined by standard matrix manipulations (Table 3). Coefficients of the matrices are obtained by multiplication of the second derivatives of energy functions and first derivatives of corresponding yield functions. An advantage of the thermomechanical formulation, is that the incremental response can be derived solely by applying standard procedures (Houlsby & Puzrin, 1999), and there is no need for either *ad hoc* procedures or additional assumptions.

	$\dot{\varepsilon}_{kl}$	$\dot{\sigma}_{kl}$
$\dot{s}$	$\begin{Bmatrix}\dot{\sigma}_{ij}\\ \dot{\theta}\\ -\dot{\chi}_{ij}\\ \dot{\alpha}_{ij}\\ \lambda\end{Bmatrix}=[U]\begin{Bmatrix}\dot{\varepsilon}_{kl}\\ \dot{s}\end{Bmatrix}$	$\begin{Bmatrix}-\dot{\varepsilon}_{ij}\\ \dot{\theta}\\ -\dot{\chi}_{ij}\\ \dot{\alpha}_{ij}\\ \lambda\end{Bmatrix}=[H]\begin{Bmatrix}\dot{\sigma}_{kl}\\ \dot{s}\end{Bmatrix}$
$\dot{\theta}$	$\begin{Bmatrix}\dot{\sigma}_{ij}\\ -\dot{s}\\ -\dot{\chi}_{ij}\\ \dot{\alpha}_{ij}\\ \lambda\end{Bmatrix}=[F]\begin{Bmatrix}\dot{\varepsilon}_{kl}\\ \dot{\theta}\end{Bmatrix}$	$\begin{Bmatrix}-\dot{\varepsilon}_{ij}\\ -\dot{s}\\ -\dot{\chi}_{ij}\\ \dot{\alpha}_{ij}\\ \lambda\end{Bmatrix}=[G]\begin{Bmatrix}\dot{\sigma}_{kl}\\ \dot{\theta}\end{Bmatrix}$

Table 3. Energy function for small strain continuum mechanics.

3 Computational Examples

The straightforwardness of the approach described above allowed a computational tool, written in the Mathematica computing environment, to be developed for implementing constitutive models. The tool is capable of predicting the entire stress-strain response of a material subject to a specified sequence of stress or strain increments. The material model is specified solely by the expressions for Gibbs or Helmholtz free energy, and the corresponding yield surface. All the differentials are evaluated by symbolical differentiation. The program is entirely successful in predicting the response of those elastic-plastic materials implemented to date.

The example presented here is that of the Modified Cam Clay model. The Modified Cam-Clay model was slightly altered to satisfy thermodynamic principles (Collins & Houlsby, 1997). The first case is the prediction of an undrained triaxial test. For this case the Helmholtz free energy approach is used as the strains are specified and stresses calculated. The necessary functions are shown in Figure 2. The stress-strain curve for an undrained loading of a normally-consolidated specimen (including an unload-reload cycle) is shown in Figure 3, and the corresponding stress path in Figure 4, where it can be seen that the path approaches the critical state line.

$$\mathrm{y}[\chi\_,\ \epsilon\_,\ \alpha\_] := 3\,\mathrm{J2}[\chi] - \frac{M^2\,\mathrm{I1}[\chi]}{3}\left(2\,\mathrm{pxo}\,\mathrm{Exp}\left[\frac{\mathrm{I1}[\alpha]}{\lambda\mathrm{star} - \kappa\mathrm{star}}\right] - \frac{\mathrm{I1}[\chi]}{3}\right);$$

$$\mathrm{f}[\epsilon\_,\ \alpha\_] := \mathrm{po}\,\kappa\mathrm{star}\,\mathrm{Exp}\left[\frac{\mathrm{I1a}[\epsilon,\alpha]}{\kappa\mathrm{star}}\right] + 2\,\mathrm{G}\,\mathrm{J2a}[\epsilon,\alpha];$$

Fig. 2. Specification of Modified Cam Clay in MATHEMATICA (*f*–formulation)

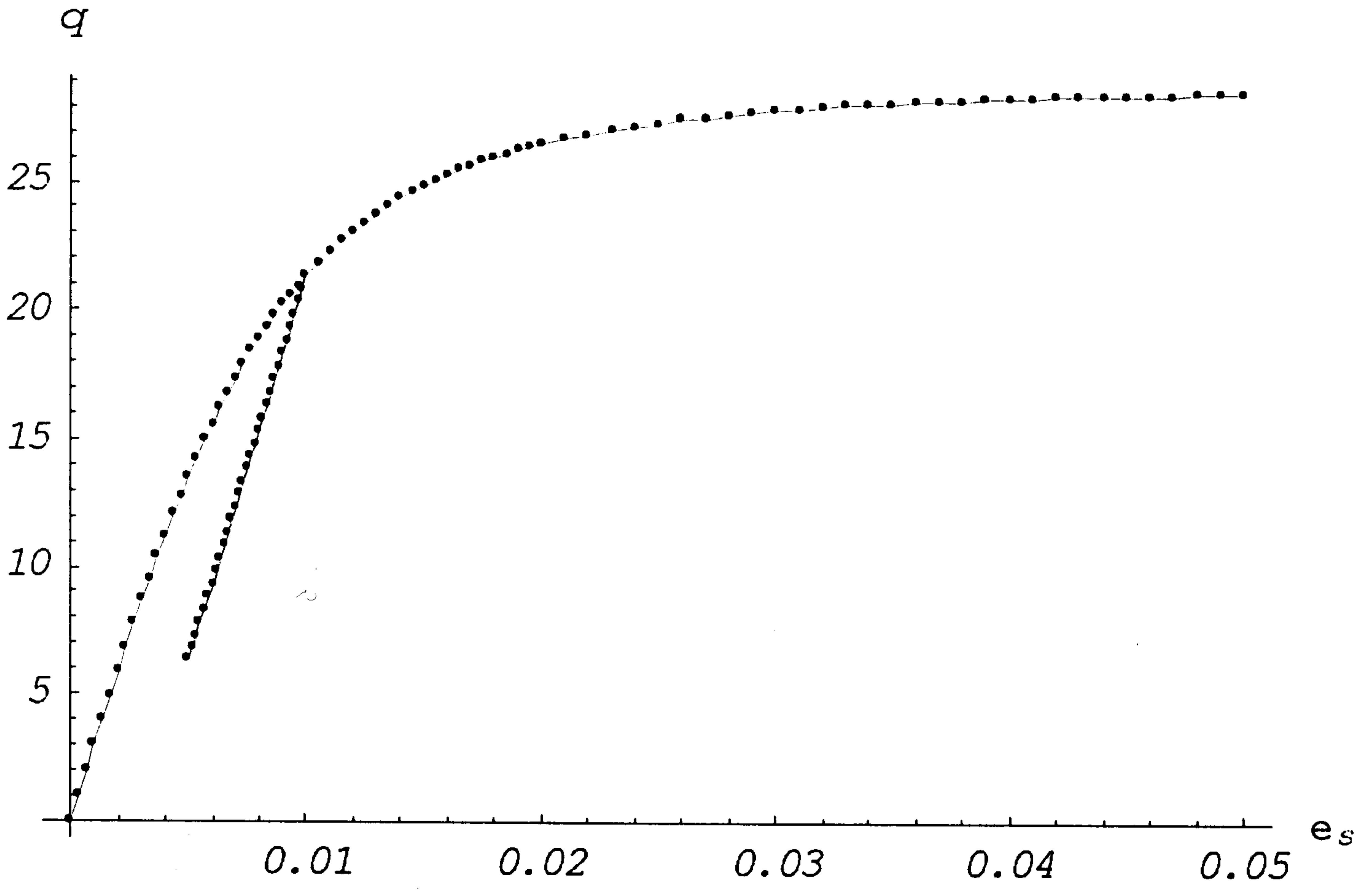


Fig. 3. Stress–strain curve for undrained test on Modified Cam Clay

The second example is the behaviour of the Modified Cam-Clay model under a cycle of stress in a drained triaxial test, and calculated in Gibbs free energy formulation. The relevant two lines within the Mathematica program to specify the model are given in Figure 5. The stress-strain curve for a stress-controlled drained test with unloading (into the triaxial extension range) followed by reloading is shown in Figure 6.

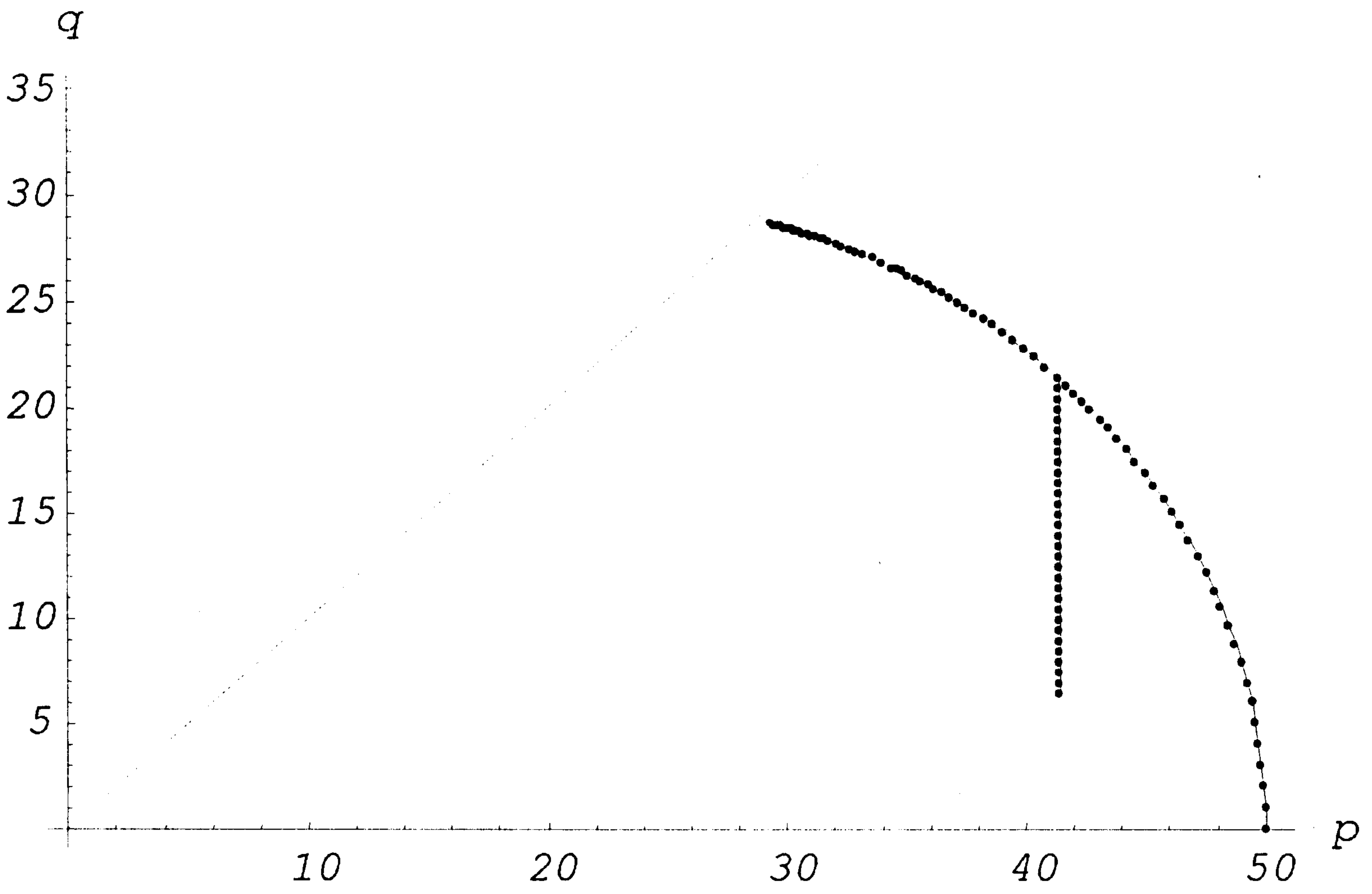


Fig. 4. Stress path for undrained test on Modified Cam Clay

$$\texttt{Y}[\chi\_,\ \sigma\_,\ \alpha\_] := 3\,\texttt{J2}[\chi] - \frac{\texttt{M}^2\,\texttt{I1}[\chi]}{3}\left(2\,\texttt{pxo}\,\texttt{Exp}\left[\frac{\texttt{I1}[\alpha]}{\lambda\texttt{star} - \texttt{xstar}}\right] - \frac{\texttt{I1}[\chi]}{3}\right);$$
$$\texttt{g}[\sigma\_,\ \alpha\_] := -\texttt{xstar}\,\frac{\texttt{I1}[\sigma]}{3}\left(\texttt{Log}\left[\frac{\texttt{I1}[\sigma]}{3\,\texttt{po}}\right] - 1\right) - \frac{\texttt{J2}[\sigma]}{2\,\texttt{G}} - \texttt{dotprod}[\sigma,\ \alpha];$$

Fig. 5. Specification of Modified Cam Clay in MATHEMATICA (g–formulation)

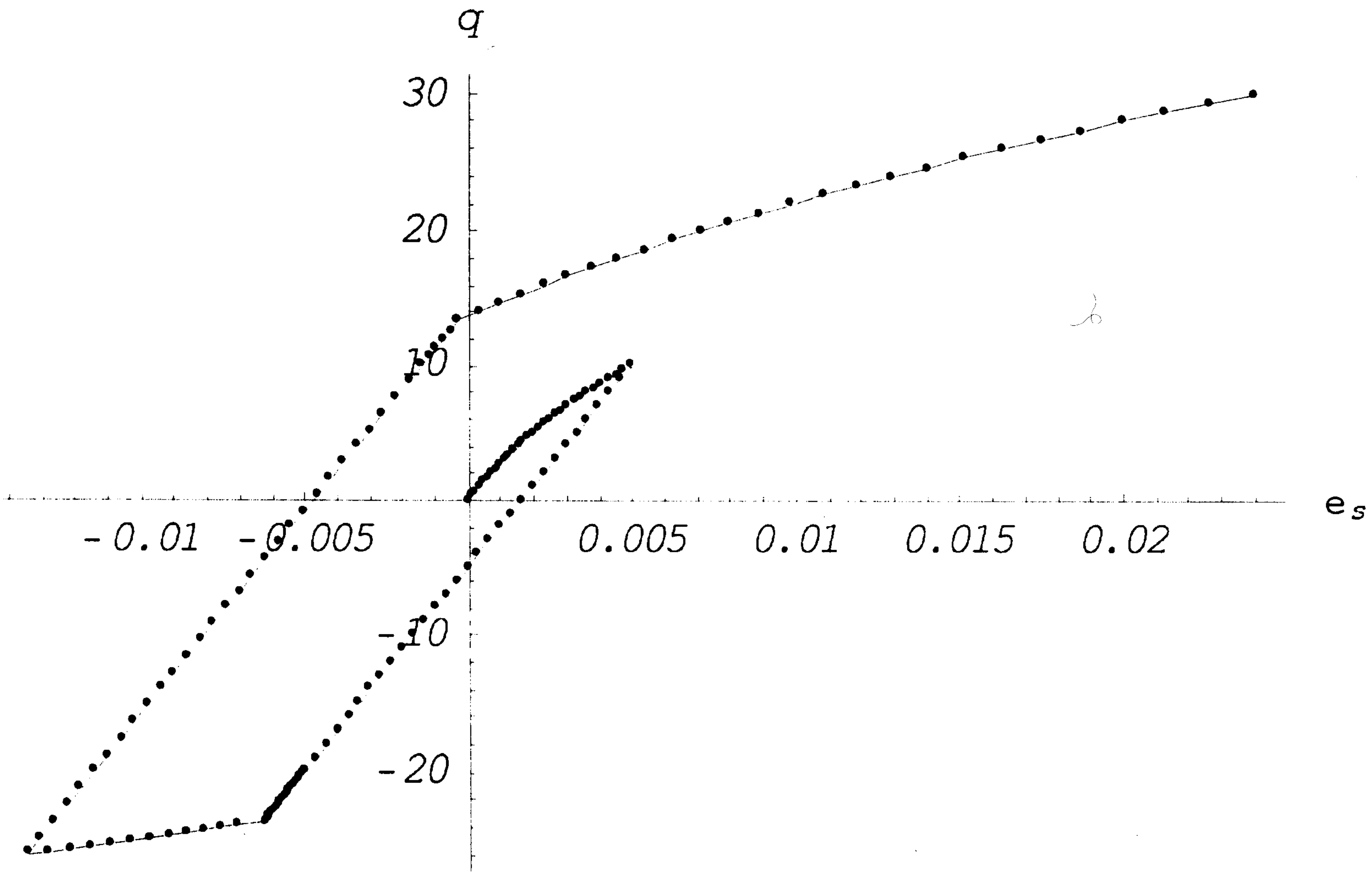
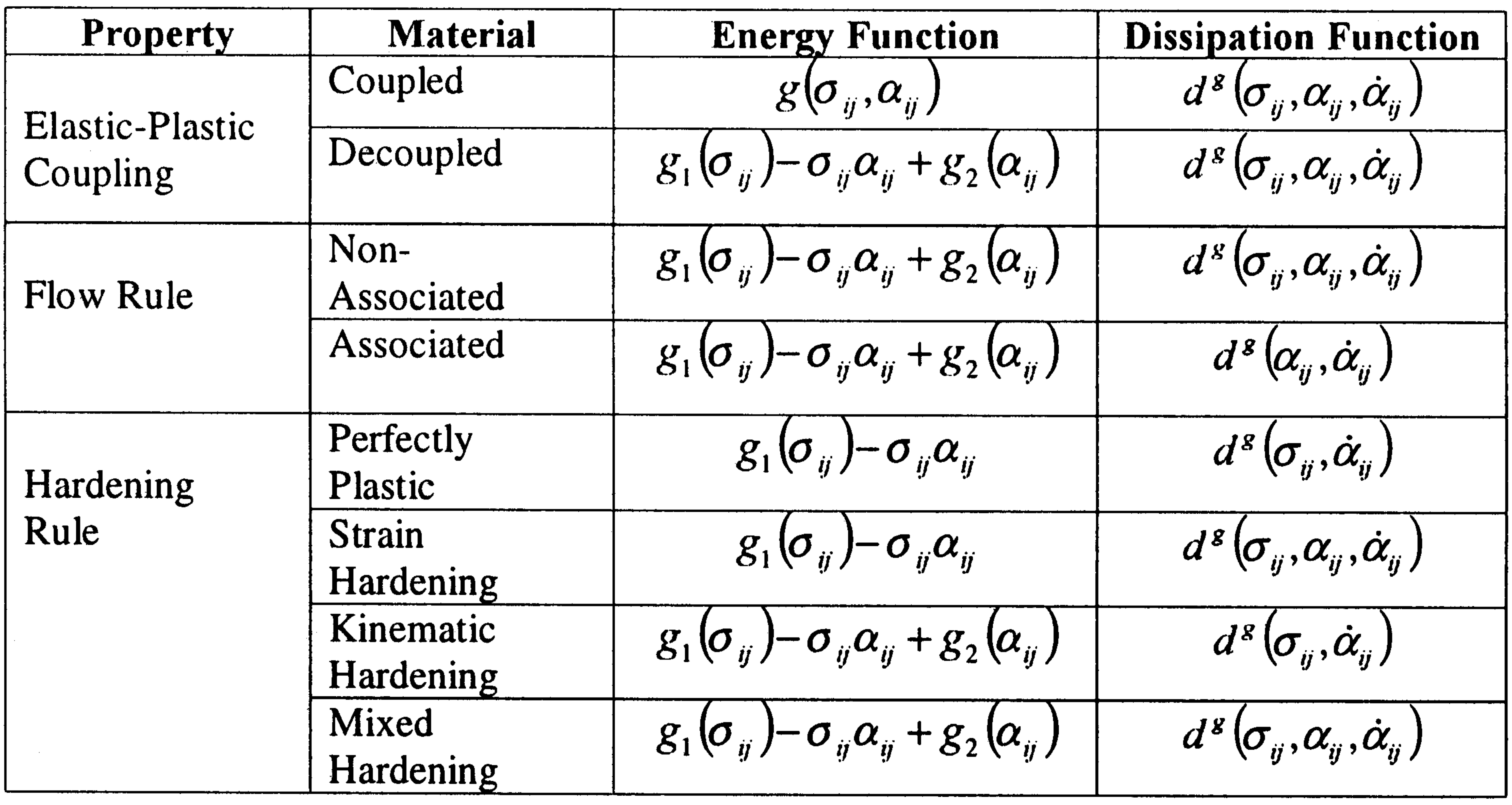


Fig. 6. Drained triaxial test on Modified Cam Clay

One of our objectives was to create a compact and consistent framework for constitutive modeling, and the computational tool described above offers this framework. An indication of this is the simplicity with which the models can be compared and new models developed within this framework. Consider, for example, a classification of the models based on the form of their potential functions.

4 Classification of plasticity models

A classification of plasticity models within the thermomechanical framework is given in Table 4. A Gibbs free energy formulation for isothermal conditions is taken as an example.



Property	Material	Energy Function	Dissipation Function
Elastic-Plastic Coupling	Coupled	$g(\sigma_{ij},\alpha_{ij})$	$d^g(\sigma_{ij},\alpha_{ij},\dot{\alpha}_{ij})$
	Decoupled	$g_1(\sigma_{ij})-\sigma_{ij}\alpha_{ij}+g_2(\alpha_{ij})$	$d^g(\sigma_{ij},\alpha_{ij},\dot{\alpha}_{ij})$
Flow Rule	Non-Associated	$g_1(\sigma_{ij})-\sigma_{ij}\alpha_{ij}+g_2(\alpha_{ij})$	$d^g(\sigma_{ij},\alpha_{ij},\dot{\alpha}_{ij})$
	Associated	$g_1(\sigma_{ij})-\sigma_{ij}\alpha_{ij}+g_2(\alpha_{ij})$	$d^g(\alpha_{ij},\dot{\alpha}_{ij})$
Hardening Rule	Perfectly Plastic	$g_1(\sigma_{ij})-\sigma_{ij}\alpha_{ij}$	$d^g(\sigma_{ij},\dot{\alpha}_{ij})$
	Strain Hardening	$g_1(\sigma_{ij})-\sigma_{ij}\alpha_{ij}$	$d^g(\sigma_{ij},\alpha_{ij},\dot{\alpha}_{ij})$
	Kinematic Hardening	$g_1(\sigma_{ij})-\sigma_{ij}\alpha_{ij}+g_2(\alpha_{ij})$	$d^g(\sigma_{ij},\dot{\alpha}_{ij})$
	Mixed Hardening	$g_1(\sigma_{ij})-\sigma_{ij}\alpha_{ij}+g_2(\alpha_{ij})$	$d^g(\sigma_{ij},\alpha_{ij},\dot{\alpha}_{ij})$

Table 4. Classification of constitutive behaviour

Let us start with classification with respect to elastic-plastic coupling. The material is decoupled, when the energy function can be presented as a sum of the following three terms: g_1 depends on stress only, g_2 depends on internal variable and a mixed term is the product of stress and internal variable tensors.

Considering further only decoupled materials, let us investigate the flow rule classification. The associated flow requires the dissipation function to be independent of stress. In other words, when the dissipation function does depend on stress, as for frictional materials, normality in stress space is impossible.

Finally, consider a classification for hardening. In perfectly plastic materials the third term in the Gibbs free energy function vanishes while the dissipation function should be independent of the internal variable. Strain hardening again omits the third term of the Gibbs free energy, but requires the dissipation function to depend on the internal variable. Kinematic hardening, on the contrary, leaves the dissipation function independent of the internal variable but requires all three terms in the Gibbs free energy function. Finally, mixed kinematic and isotropic hardening requires both the three terms in the Gibbs free energy function and the dependency of the dissipation function on the internal variable. As is seen, this simple classification covers the most important cases of conventional plasticity.

In fact, generalisation of this framework (Puzrin & Houlsby 1999) allows for even broader classes of modern plasticity models to be derived using the thermomechanical approach. First, introduction of multiple kinematic internal variables leads to the thermomechanical formulation of the kinematic hardening plasticity with multiple yield surfaces. The next step of generalization was to introduce continuous internal functions in stead of a discrete set of internal variables. However, this was a significant step forward, because it required a reformulation of the complete thermomechanical framework in terms of energy and dissipation functionals instead of functions. Fortunately, utilization of Frechet differentials and Legendre transforms of functionals made this reformulation quite straightforward. A direct application of this generalization is the thermomechanical formulation of the kinematic hardening plasticity with infinite number of yield surfaces.

5 Conclusions

Subject to some restrictions, the proposed thermomechanical framework for constitutive modeling contains conventional plasticity as a subset. These restrictions are weak enough to allow for some forms of non-associated flow and concavity of the yield surface, but on the other hand they are sufficiently strict to ensure that a constitutive model satisfies the Laws of Thermodynamics. At the same time the proposed framework appeared to be very compact and consistent, allowing for simple classification and development of constitutive models. To investigate the possibilities offered by this new approach, further extensive research is required.

An obvious step forward would be generalization of the computational tool to include the multiple variables and functional version. This would allow for further investigation of existing models and development of new ones. A very important step would be incorporation of this computational tool into a Finite Element code to study directly the effects of potential functions on the solution of boundary value problems. The theory itself requires further generalisation to incorporate rate dependency and more general forms of material memory.

Finally, we have not yet addressed our final objective: the Uniqueness and Bounds Theorems. An advantage of the proposed framework is that it makes considerable use of potential functions. The use of potentials is closely related to variational and extremum principles. This offers the possibility of deriving more general theorems about the constitutive models or, at least, of establishing the range of applicability of the existing ones.

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