

The Framework of Thermodynamics Approach to Constitutive Modelling

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1 General concept

1.1 Strain

We are assuming small deformation theory, so that strains are described by the small strain tensor ε_{ij} , and the deformation rate tensor is equal to its rate of change $\dot{\varepsilon}_{ij}$

1.2 Stress

Stresses are defined so that the power of deformation per unit volume is $\sigma_{ij}\dot{\varepsilon}_{ij}$

1.3 State

The state of a material element is defined by ε_{ij} , an internal variable α_{ij} and either temperature θ or entropy S . For the present purposes, it is sufficient to introduce a single second order tensorial internal variable, which can frequently be identified with the "plastic strain"

2 Thermodynamics laws

First law:

$$\dot{W} + \dot{Q} = \dot{U} \quad (1)$$

Second law:

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

in which:

- $\dot{W} = \sigma_{ij}\dot{\varepsilon}_{ij}$: mechanical work input
- $\dot{Q} = -q_{k,k}$: heat supply to a volume element
- q_k : heat flux vector
- $U(\varepsilon_{ij}, \alpha_{ij}, S)$: internal energy per unit volume
- S : entropy
- $\frac{q_k}{\theta}$: entropy flux

Expansion of equation (2) gives us:

$$\dot{S} \geq -\frac{q_{k,k}\theta - q_k\theta_{,k}}{\theta^2} \quad (3)$$

$$\theta\dot{S} + q_{k,k} - \frac{q_k\theta_{,k}}{\theta} \geq 0 \quad (4)$$

The first two terms $\theta\dot{S} + q_{k,k} = \dot{D}$ are called mechanical dissipation. The third term $-q_k\theta_{,k}/\theta$ is called thermal dissipation. The thermal dissipation is always non-negative by virtue of the fact that the heat flux is always in the direction of the negative thermal gradient. The third term becomes small by comparison with the first two for slow process, so it is argued that the mechanical dissipation must itself be non-negative. Required both $\theta\dot{S} + q_{k,k} = \dot{D} \geq 0$ and $-q_k\theta_{,k}/\theta \geq 0$ is more stringent condition than the second law, but it is widely accepted. In this case the separation of the thermal and mechanical dissipations and enforcement of the mechanical dissipation should only be considered as a restriction on the field of continua treated in this study. In the following, we shall require that $\dot{D} \geq 0$

From (1) $\Rightarrow \dot{U} = \sigma_{ij}\dot{\varepsilon}_{ij} - q_{k,k}$, and the definition of \dot{D} it follows that:

$$\dot{U} = \sigma_{ij}\dot{\varepsilon}_{ij} + \theta\dot{S} - \dot{D} \quad (5)$$

The internal energy is a function of the state. In writing this function, it is convenient to choose the entropy rather than the temperature as the independent variable so that we write $U = U(\varepsilon_{ij}, \alpha_{ij}, S)$

Furthermore, the time derivative of internal energy U :

$$\dot{U} = \frac{\partial U}{\partial \varepsilon_{ij}} \dot{\varepsilon}_{ij} + \frac{\partial U}{\partial \alpha_{ij}} \dot{\alpha}_{ij} + \frac{\partial U}{\partial S} \dot{S} \quad (6)$$

Comparing eq(5) and eq(6), we can derive these relationships:

$$\sigma_{ij} = \frac{\partial U}{\partial \varepsilon_{ij}} \quad (7)$$

$$\theta = \frac{\partial U}{\partial S} \quad (8)$$

$$\dot{D} = -\frac{\partial U}{\partial \alpha_{ij}} \dot{\alpha}_{ij} \quad (9)$$

It can be seen here that the associated variables with strain ε_{ij} and temperature θ are stress σ_{ij} and entropy S , respectively. Therefore, in an analogous manner, the thermodynamic forces associated with the internal variable α_{ij} can be defined to be:

$$\bar{\chi}_{ij} = -\frac{\partial U}{\partial \alpha_{ij}} \quad (10)$$

$\bar{\chi}$ is a stress-like variable, and it is called the generalized stress. Now, the dissipation function can be rewritten as follow:

$$\dot{D} = \bar{\chi}_{ij} \dot{\alpha}_{ij} \quad (11)$$

We assume that the dissipation function is not only a function of the thermodynamic state of the material, but also the rate of the state. It is found, in the following that it is sufficient to consider just those mechanisms where dissipation depends only on the rate of change of the internal variable $\dot{\alpha}_{ij}$.

The dissipation function can be written in various forms:

$$\begin{aligned} \dot{D} &= \dot{D}^F = \dot{D}(\varepsilon_{ij}, \alpha_{ij}, \dot{\alpha}_{ij}) \\ \dot{D} &= \dot{D}^G = \dot{D}(\sigma_{ij}, \alpha_{ij}, \dot{\alpha}_{ij}) \end{aligned}$$

In each case, we define "dissipative generalized stress" as $\chi_{ij} = \partial \dot{D}^E / \partial \dot{\alpha}_{ij}$, with E stands for G or F

Using the fact that for a rate-independent material, the dissipation \dot{D} must be a homogeneous of degree one in the rate $\dot{\alpha}_{ij}$ (Houlsby and Puzrin, 2000). Euler's theorem gives:

$$\dot{D} = \frac{\partial \dot{D}}{\partial \dot{\alpha}_{ij}} \dot{\alpha}_{ij} = \chi_{ij} \dot{\alpha}_{ij} \quad (12)$$

NOTE: the reason why dissipation must be a homogeneous of degree one in the rate of internal variables can be explained in this way: The differentiate of dissipation function gives the dissipative generalized stress. This dissipative generalized stress will appear in our constitutive model. If dissipation function is not the first order homogeneous, the transformation from the function of internal variable (dissipation function) to the function of dissipative stress (yield stress), the internal variable which is contained in dissipative stress cannot be fully eliminated. Thus, the model will be rate-dependent. In other words, if dissipation function is not the first order homogeneous, it will lead to the yield function for rate-independent material

Comparing (11) and (12), one obtains:

$$(\bar{\chi}_{ij} - \chi_{ij}) \dot{\alpha}_{ij} = 0 \quad (13)$$

As χ_{ij} may be a function of $\dot{\alpha}_{ij}$, it can be concluded here that $\bar{\chi}_{ij} - \chi_{ij}$ is always orthogonal to $\dot{\alpha}_{ij}$. However, as argued by Ziegler (1983) and presented by Houlsby and Puzrin (2000), a rather wide range of classes of materials can be described by enforcement of a stronger condition $\bar{\chi}_{ij} = \chi_{ij}$. This condition is called Ziegler's orthogonality condition and was adopted in the framework by Houlsby and Puzrin (2000)

3 An approach by Helmholtz specific free energy $F(\varepsilon_{ij}, \alpha_{ij}, \theta)$

Since we are concerned with isothermal deformation in which θ is constant, it will be more convenient if S is replaced by θ in the expression for energy function. Notice that $\sigma_{ij} = \partial U / \partial S$. Therefore, the internal energy $U(\varepsilon_{ij}, \alpha_{ij}, S)$ can be transformed into the function $F(\varepsilon_{ij}, \alpha_{ij}, \theta)$ by using Legendre transformation.

$$U - F = S\theta \Rightarrow F = U - S\theta \quad (14)$$

in which: $S = -\partial F / \partial \theta$. Differentiate F with respect to time results in:

$$\dot{F} = \dot{U} - \dot{S}\theta - \theta\dot{S} \quad (15)$$

From eq (5) and (15)

$$\dot{D} = \sigma_{ij}\dot{\varepsilon}_{ij} - \dot{F} - \dot{\theta}S - \frac{q_k\theta_{,k}}{\theta} \geq 0 \quad (16)$$

As explained in the previous part, $-q_k\theta_{,k}/\theta$ is negative and small, therefore; it is neglected. Thus, the rate of dissipation function can be rewritten:

$$\dot{D} = \sigma_{ij}\dot{\varepsilon}_{ij} - \dot{F} - \dot{\theta}S \geq 0 \quad (17)$$

If the isothermal problems are considered, then \dot{D} is simplified into:

$$\dot{D} = \sigma_{ij}\dot{\varepsilon}_{ij} - \dot{F} \quad (18)$$

4 Gibbs Free Energy Function

For further developments, it has been proved convenient to also introduce the Gibbs free energy function $G(\sigma_{ij}, \alpha_{ij})$. This can be obtained from the Helmholtz free energy function $F(\varepsilon_{ij}, \alpha_{ij})$, by a partial Legendre transformation interchanging the strain and stress variables:

$$F(\varepsilon_{ij}, \alpha_{ij}) - G(\sigma_{ij}, \alpha_{ij}) = \sigma_{ij}\varepsilon_{ij} \quad (19)$$

where:

$$\varepsilon_{ij} = -\frac{\partial G}{\partial \sigma_{ij}} \quad (20)$$

and

$$\chi_{ij} = -\frac{\partial G}{\partial \alpha_{ij}} \quad (21)$$

5 Thermodynamics potentials for elastic/plastic materials

5.1 Decouple materials

In developments of the theory of elasto-plastic materials it is common to assume at the outset that the (small) strain tensor can be regarded as the sum of "elastic" and "plastic" parts. However, it is possible to deduce this decomposition formally for a material whose instantaneous elastic moduli are independent of the internal variables - a so called "decoupled material"

Differentiating (20) with respect to time shows that the strain rate is the sum of two terms:

$$\dot{\varepsilon}_{ij} = -\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} \dot{\sigma}_{kl} - \frac{\partial^2 G}{\partial \sigma_{ij} \partial \alpha_{kl}} \dot{\alpha}_{kl} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^p \quad (22)$$

The coefficient of the $\dot{\sigma}_{kl}$ term is the instantaneous elastic compliance, which, for a decouple material, is independent of the internal variable α_{ij} , so that $\frac{\partial^3 G}{\partial \sigma_{ij} \partial \sigma_{kl} \partial \sigma_{mn}} = 0$

It follows that the coefficient of the $\dot{\alpha}_{ij}$ term is necessary independent of σ_{ij} . Hence, both terms can be integrated separately with respect to time to give the elastic strain, and plastic strain, respectively.

It further follows from the decoupled assumption, upon integration of the second derivatives in (22) that the Gibbs free energy function must take the form

$$G(\sigma_{ij}, \alpha_{ij}) = G_1(\sigma_{ij}) + G_3(\alpha_{ij})\sigma_{ij} + G_2(\alpha_{ij}) \quad (23)$$

The cross term is hence linear in stress. Up to this point, the internal variable has not been given any specific physical significance.

We can replace the function $G_3(\alpha_{ij})$ by α_{ij} without any loss of generality:

$$G(\sigma_{ij}, \alpha_{ij}) = G_1(\sigma_{ij}) - \sigma_{ij}\alpha_{ij} + G_2(\alpha_{ij}) \quad (24)$$

From (20):

$$\varepsilon_{ij} = -\frac{\partial G}{\partial \sigma_{ij}} = -\frac{\partial G_1}{\partial \sigma_{ij}}(\sigma_{ij}) + \alpha_{ij} \quad (25)$$

or:

$$\varepsilon_{ij} = \varepsilon_{ij}^e(\sigma_{ij}) + \alpha_{ij} \quad (26)$$

where the elastic strain ε_{ij}^e is a function just of stress and α_{ij} can now be identified as the plastic strain.

With this choice of α , the mixed second derivative $\frac{\partial^2 G}{\partial \sigma_{ij} \partial \alpha_{kl}} = -\delta_{ik}\delta_{jl}$

5.2 Couple material

6 Derived Yield Function and Flow Rule from Dissipation function

6.1 Singular transformation of a first order homogeneous function

The transformation from a homogeneous of degree one function $X(x_i, \alpha_i)$ to the function $Y(y_i, \alpha_i)$ is considered in this section. In the practical problem, X stands for dissipation function with x is the internal variable; while Y represents the yield function with y is the dissipative generalized stress.

Legendre transformation:

$$X(x_i, \alpha_i) + Y(y_i, \alpha_i) = x_i y_i \quad (27)$$

in which:

$$x_i = \frac{\partial Y}{\partial y_i} \quad (28)$$

$$y_i = \frac{\partial X}{\partial x_i} \quad (29)$$

Because $X(x_i, \alpha_i)$ is a homogeneous of degree one function, we have:

$$X(x_i, \alpha_i) = x_i \frac{\partial X}{\partial x_i} \quad (30)$$

From eq(27) and eq(30)

$$Y(y_i, \alpha_i) = 0 \quad (31)$$

From this point we can see that the value of the function Y is always 0

From (27) and (31):

$$\begin{aligned} x_i y_i &= X(x_i, \alpha_i) \\ x_i dy_i + y_i dx_i &= \frac{\partial X}{\partial x_i} dx_i + \frac{\partial X}{\partial \alpha_i} d\alpha_i \\ x_i dy_i + y_i dx_i &= y_i dx_i + \frac{\partial X}{\partial \alpha_i} d\alpha_i \end{aligned}$$

Therefore:

$$x_i dy_i - \frac{\partial X}{\partial \alpha_i} d\alpha_i = 0 \quad (32)$$

The differentiation of the dual function $Y(y_i, \alpha_i) = 0$ gives:

$$\frac{\partial Y}{\partial y_i} dy_i + \frac{\partial Y}{\partial \alpha_i} d\alpha_i = 0 \quad (33)$$

From (32) and (33):

$$x_i = \Lambda \frac{\partial Y}{\partial y_i} \quad (34)$$

$$\Lambda \frac{\partial Y}{\partial \alpha_i} = -\frac{\partial X}{\partial \alpha_i} \quad (35)$$

Note:

- a) λ is an undetermined scalar, reflecting the non-unique nature of this singular transformation
- b) The value of $y_i = \partial X / \partial x_i$ is unaffected by the transformation $x_i \rightarrow \lambda x_i$. So, the mapping from $x_i \rightarrow y_i$ is $\infty \rightarrow 1$

6.2 Derive the flow rule and yield function from a stress-independent dissipation function

Consider dissipation functions which depend only on α_{ij} and $\dot{\alpha}_{ij}$. Other possible functional dependencies will be discussed later. Also, we only consider rate-independent material here, which means the dissipation function D must be homogeneous of degree one in $\dot{\alpha}_{ij}$.

From the orthogonality postulate, it follows that the generalized stresses are given by:

$$\chi_{ij} = \frac{\partial \dot{D}}{\partial \dot{\alpha}_{ij}}(\alpha_{ij}, \dot{\alpha}_{ij}) \quad (36)$$

So that, in general, a Legendre Transformation of $\dot{D}(\alpha_{ij}, \dot{\alpha}_{ij})$ introduces a new function $\Omega(\alpha_{ij}, \chi_{ij})$, with the properties that

$$\dot{D}(\alpha_{ij}, \dot{\alpha}_{ij}) + \Omega(\alpha_{ij}, \chi_{ij}) = \chi_{ij} \dot{\alpha}_{ij} \quad (37)$$

From the Legendre transformation for a singular transformation of a homogeneous of degree one as discussed above, we can derive a function that contains only stress-like variable, and that the value of that function is always zero, which is the same characteristic to the yield function

$$f(\alpha_{ij}, \chi_{ij}) = 0 \quad (38)$$

and the flow rule:

$$\dot{\alpha}_{ij} = \Lambda \frac{\partial f}{\partial \chi_{ij}} \quad (39)$$

Equation (39) are associated flow rule, expressed in generalized stress space, not true stress space.

The question immediately arises "does normality also hold in true stress space?" To answer this question, we must replace χ_{ij} in eq (39) by σ_{ij} .

A field function in true stress space can be defined by:

$$\hat{f}(\alpha_{ij}, \sigma_{ij}) = f(\alpha_{ij}, -\frac{\partial G}{\partial \alpha_{ij}}(\sigma_{ij}, \alpha_{ij})) = 0 \quad (40)$$

Then

$$\frac{\partial \hat{f}}{\partial \sigma_{ij}} = \frac{\partial f}{\partial \chi_{kl}} \frac{-\partial^2 G}{\partial \alpha_{kl} \partial \sigma_{ij}} \quad (41)$$

so that the flow rule now takes the form:

$$\Lambda \frac{\partial \hat{f}}{\partial \sigma_{ij}} = \frac{-\partial^2 G}{\partial \alpha_{kl} \partial \sigma_{ij}} \dot{\alpha}_{kl} \quad (42)$$

From eq(22) and (42):

$$\varepsilon_{ij}^p = \Lambda \frac{\partial \hat{f}}{\partial \sigma_{ij}} \quad (43)$$

To sum up, if the internal variable is chosen to be plastic strain ε_{ij}^p then, the associated flow rule is satisfied in both true stress and dissipative generalized stress space as long as dissipation function is not stress-dependent function

6.3 Derive the flow rule and yield function from a stress-dependent dissipation function

Consider the dissipation functions of the form $\dot{D}(\sigma_{ij}, \alpha_{ij}, \dot{\alpha}_{ij})$.

From the orthogonality postulate, it follows that the generalized stresses are given by:

$$\chi_{ij} = \frac{\partial \dot{D}}{\partial \dot{\alpha}_{ij}}(\sigma_{ij}, \alpha_{ij}, \dot{\alpha}_{ij}) \quad (44)$$

So that, in general, a Legendre Transformation of $\dot{D}(\sigma_{ij}, \alpha_{ij}, \dot{\alpha}_{ij})$ to a new function $\Omega(\sigma_{ij}, \alpha_{ij}, \chi_{ij})$, with the properties that

$$\dot{D}(\sigma_{ij}, \alpha_{ij}, \dot{\alpha}_{ij}) + \Omega(\sigma_{ij}, \alpha_{ij}, \chi_{ij}) = \chi_{ij} \dot{\alpha}_{ij} \quad (45)$$

From the Legendre transformation for a singular transformation of a homogeneous of degree one as discussed above, we derive a function in which its value is always zero, which is same characteristic to the yield function:

$$f(\sigma_{ij}, \alpha_{ij}, \chi_{ij}) = 0 \quad (46)$$

and this relationship, which is identity to flow rule:

$$\dot{\alpha}_{ij} = \Lambda \frac{\partial f}{\partial \chi_{ij}} \quad (47)$$

$$\frac{\partial D}{\partial \sigma_{ij}} = -\Lambda \frac{\partial f}{\partial \sigma_{ij}} \quad (48)$$

and for passive variables:

$$\frac{\partial D}{\partial \alpha_{ij}} = -\Lambda \frac{\partial f}{\partial \alpha_{ij}} \quad (49)$$

Equation (47) are associated flow rule, expressed in generalized stress space, not true stress space.

The question immediately arises "does normality also hold in true stress space?" To answer this question, we must replace χ_{ij} in eq (47) by σ_{ij} .

A field function in true stress space can be defined by:

$$\hat{f}(\alpha_{ij}, \sigma_{ij}) = f(\sigma_{ij}, \alpha_{ij}, \frac{-\partial G}{\partial \alpha_{ij}}(\sigma_{ij}, \alpha_{ij})) = 0 \quad (50)$$

Then

$$\frac{\partial \hat{f}}{\partial \sigma_{ij}} = \frac{\partial f}{\partial \sigma_{ij}} + \frac{\partial f}{\partial \chi_{kl}} \frac{-\partial^2 G}{\partial \alpha_{kl} \partial \sigma_{ij}} \quad (51)$$

So that the flow rule now takes the form:

$$\Lambda \frac{\partial \hat{f}}{\partial \sigma_{ij}} = \Lambda \frac{\partial f}{\partial \sigma_{ij}} + \frac{-\partial^2 G}{\partial \alpha_{kl} \partial \sigma_{ij}} \dot{\alpha}_{kl} \quad (52)$$

From eq(22), (52) and (48):

$$\varepsilon_{ij}^p = \Lambda \frac{\partial \hat{f}}{\partial \sigma_{ij}} + \frac{\partial \dot{D}}{\partial \sigma_{ij}} \quad (53)$$

We have noticed that when \dot{D} depends explicitly on the stress, the normality rule cannot be expected to hold in true stress space. As for the case of coupled material it is to be emphasised that this non-associated behavior arises naturally from the general thermomechanical framework, no new function needs to be introduced to describe to formulate the constitutive equations

7 Elastoplastic stiffness matrix Dep

The increment form of strain from (22)

$$\varepsilon_{ij} = -\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} \dot{\sigma}_{kl} - \frac{\partial^2 G}{\partial \sigma_{ij} \partial \alpha_{kl}^p} \dot{\alpha}_{kl}^p \quad (54)$$

Associated flow rule for rate-independent material (43):

$$\dot{\alpha}_{kl}^p = \Lambda \frac{\partial \hat{f}}{\partial \sigma_{kl}} \quad (55)$$

From the yield function in(46), consistency condition is derived:

$$\dot{\hat{f}} = \frac{\partial \hat{f}}{\partial \sigma_{mn}} \dot{\sigma}_{mn} + \frac{\partial \hat{f}}{\partial \alpha_{ij}} \dot{\alpha}_{ij} = 0 \quad (56)$$

$$\dot{\hat{f}} = \frac{\partial \hat{f}}{\partial \sigma_{mn}} \dot{\sigma}_{mn} + \frac{\partial \hat{f}}{\partial \alpha_{mn}} \Lambda \frac{\partial \hat{f}}{\partial \sigma_{mn}} \quad (57)$$

Thus, plastic multiplier is calculated as follow:

$$\Lambda = \frac{-\frac{\partial \hat{f}}{\partial \sigma_{mn}} \dot{\sigma}_{mn}}{\frac{\partial \hat{f}}{\partial \alpha_{mn}} \frac{\partial \hat{f}}{\partial \sigma_{mn}}} \quad (58)$$

We substitute this into equation (54)

$$\dot{\varepsilon}_{ij} = -\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} \dot{\sigma}_{kl} - \frac{\partial^2 G}{\partial \sigma_{ij} \partial \alpha_{kl}} \Lambda \frac{\partial \hat{f}}{\partial \sigma_{kl}} \quad (59)$$

$$\dot{\varepsilon}_{ij} = -\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} \dot{\sigma}_{kl} - \frac{\partial^2 G}{\partial \sigma_{ij} \partial \alpha_{kl}} \frac{-\frac{\partial \hat{f}}{\partial \sigma_{mn}} \dot{\sigma}_{mn}}{\frac{\partial \hat{f}}{\partial \alpha_{mn}} \frac{\partial \hat{f}}{\partial \sigma_{mn}}} \frac{\partial \hat{f}}{\partial \sigma_{kl}} \quad (60)$$

$$\dot{\varepsilon}_{ij} = \left[-\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{mn}} + \frac{\frac{\partial^2 G}{\partial \sigma_{ij} \partial \alpha_{kl}} \frac{\partial \hat{f}}{\partial \sigma_{kl}}}{\frac{\partial \hat{f}}{\partial \alpha_{mn}} \frac{\partial \hat{f}}{\partial \sigma_{mn}}} \right] \dot{\sigma}_{mn} \quad (61)$$

Thus, the Elastoplastic compliance matrix is derived as follow:

$$C_{ep} = \left[-\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{mn}} + \frac{\frac{\partial^2 G}{\partial \sigma_{ij} \partial \alpha_{kl}} \frac{\partial \hat{f}}{\partial \sigma_{kl}}}{\frac{\partial \hat{f}}{\partial \alpha_{mn}} \frac{\partial \hat{f}}{\partial \sigma_{mn}}} \right] \quad (62)$$

Remember, the Elastic compliance matrix is:

$$C_e = \left[-\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{mn}} \right] \quad (63)$$

8 Application of the framework to develop Modified Cam Clay model

8.1 Two energy functions

The whole constitutive model of Modified Cam clay, which is an isotropic hardening model, will be developed based on only 2 energy functions:

a) Rate of dissipation energy

$$\dot{D} = \frac{1}{2}p_c \sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} = \pi_c \sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2}; \pi_c = \frac{p_c}{2} \quad (64)$$

in which $p_c = p_c \varepsilon_v^p$ is the maximum preconsolidation pressure. Notice that \dot{D} is a homogeneous of degree one with respect to $\dot{\varepsilon}_v^p$ and $\dot{\varepsilon}_d^p$ because we are working with a rate-independent model

b) Gibbs free energy function

$$G = -\kappa p \left(\ln \frac{p}{p_R} - 1 \right) - \frac{q^2}{6g_s} - (p\varepsilon_v^p + q\varepsilon_d^p) + \frac{1}{2}(\lambda - \kappa)p_{c0} \exp\left(\frac{\varepsilon_v^p}{\lambda - \kappa}\right) \quad (65)$$

8.2 Yield function in dissipative stress space

The Legendre transformation from a homogeneous of degree one function $\dot{D}(\dot{\varepsilon}_v^p, \dot{\varepsilon}_d^p, \pi_c)$ to a function $\Omega(\pi, \tau, \pi_c)$

Which means:

$$\dot{D} + \Omega = \pi \dot{\varepsilon}_v^p + \tau \dot{\varepsilon}_d^p \quad (66)$$

In which:

Dissipative stress:

$$\pi = \frac{\partial \dot{D}}{\partial \dot{\varepsilon}_v^p} = \pi_c \frac{\dot{\varepsilon}_v^p}{\sqrt{\dot{\varepsilon}_v^p{}^2 + M^2 \dot{\varepsilon}_d^p{}^2}}; \tau = \frac{\partial \dot{D}}{\partial \dot{\varepsilon}_d^p} = \pi_c \frac{M^2 \dot{\varepsilon}_d^p}{\sqrt{\dot{\varepsilon}_v^p{}^2 + M^2 \dot{\varepsilon}_d^p{}^2}} \quad (67)$$

From (66):

$$\begin{aligned} \Omega &= \pi \dot{\varepsilon}_v^p + \tau \dot{\varepsilon}_d^p - \pi_c \sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} \\ &= \frac{\pi^2}{\pi_c} \sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} + \frac{\tau^2}{\pi_c M^2} \sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} - \pi_c \sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} \\ &= \pi_c \sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} \left(\frac{\pi^2}{\pi_c^2} + \frac{\tau^2}{M^2 \pi_c^2} - 1 \right) \end{aligned}$$

Finally:

$$\Omega = \pi_c \sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} \left(\frac{\pi^2}{\pi_c^2} + \frac{\tau^2}{M^2 \pi_c^2} - 1 \right) \quad (68)$$

Again, because \dot{D} is the homogeneous of degree one with respect to $\dot{\varepsilon}_v^p$ and $\dot{\varepsilon}_d^p$ we directly have: $\dot{D} = \frac{\partial \dot{D}}{\partial \dot{\varepsilon}_v^p} \dot{\varepsilon}_v^p + \frac{\partial \dot{D}}{\partial \dot{\varepsilon}_d^p} \dot{\varepsilon}_d^p = \pi \dot{\varepsilon}_v^p + \tau \dot{\varepsilon}_d^p$. Therefore, Ω is equal to 0 in equation (66). Therefore, based on the formation of Ω in (68) we can derived this equation:

$$\frac{\pi^2}{\pi_c^2} + \frac{\tau^2}{M^2 \pi_c^2} = 1 \quad (69)$$

Now, we obtain a function in which its value is always zero. Therefore, we can consider it as the yield function in dissipative stress space:

$$f(\pi, \tau, \pi_c) : \frac{\pi^2}{\pi_c^2} + \frac{\tau^2}{M^2 \pi_c^2} - 1 = 0 \quad (70)$$

8.3 Flow rule in dissipative stress space

The dissipation function which is the homogeneous first order function of strain rates can now be written in this form:

$$\dot{D}(\dot{\varepsilon}_v^p, \dot{\varepsilon}_d^p, \pi_c) = \pi \dot{\varepsilon}_v^p + \tau \dot{\varepsilon}_d^p \quad (71)$$

The time derivative of both sides of equation (71) give:

$$\begin{aligned} \frac{\partial \dot{D}}{\partial \dot{\varepsilon}_v^p} d\dot{\varepsilon}_v^p + \frac{\partial \dot{D}}{\partial \dot{\varepsilon}_d^p} d\dot{\varepsilon}_d^p + \frac{\partial \dot{D}}{\partial \pi_c} d\pi_c &= \dot{\varepsilon}_v^p d\pi + \pi d\dot{\varepsilon}_v^p + \dot{\varepsilon}_d^p d\tau + \tau d\dot{\varepsilon}_d^p \\ \Leftrightarrow \pi d\dot{\varepsilon}_v^p + \tau d\dot{\varepsilon}_d^p + \frac{\partial \dot{D}}{\partial \pi_c} d\pi_c &= \dot{\varepsilon}_v^p d\pi + \pi d\dot{\varepsilon}_v^p + \dot{\varepsilon}_d^p d\tau + \tau d\dot{\varepsilon}_d^p \\ \Leftrightarrow \dot{\varepsilon}_v^p d\pi + \dot{\varepsilon}_d^p d\tau - \frac{\partial \dot{D}}{\partial \pi_c} d\pi_c &= 0 \end{aligned}$$

Finally we have:

$$\dot{\varepsilon}_v^p d\pi + \dot{\varepsilon}_d^p d\tau - \frac{\partial \dot{D}}{\partial \pi_c} d\pi_c = 0 \quad (72)$$

Consistency condition:

A mathematical expression of the requirement that the stress state stays on the failure surface as long as loading continues, even though the failure surface itself will be moving and changing shape due to hardening: $f + df = 0$ However, recall that the failure surface is defined such that $f = 0$ is the onset of plastic flow. Thus, the above equation can be simplified : $df = 0$. From (70):

$$\frac{\partial f}{\partial \pi} d\pi + \frac{\partial f}{\partial \tau} d\tau + \frac{\partial f}{\partial \pi_c} d\pi_c = 0 \quad (73)$$

From (72),(73), flow rule is obtained:

$$\dot{\varepsilon}_v^p = \Lambda \frac{\partial f}{\partial \pi}; \quad (74)$$

$$\dot{\varepsilon}_d^p = \Lambda \frac{\partial f}{\partial \tau}; \quad (75)$$

and this is also one of the result from the transformation

$$\frac{\partial \dot{D}}{\partial \pi_c} = -\Lambda \frac{\partial f}{\partial \pi_c} \quad (76)$$

Note: The flow rule is always associated in dissipative stress space.

8.4 Relationship between true stress and dissipative stress

Apply eq (21) with respect to the Gibbs free energy chosen above, we obtain:

$$\pi = -\frac{\partial G}{\partial \varepsilon_v^p} = p + p_c; \tau = -\frac{\partial G}{\partial \varepsilon_d^p} = q \quad (77)$$

In which $p_c = p_{c0} \exp\left(\frac{\varepsilon_v^p}{\lambda - \kappa}\right)$ is the maximum pre-consolidation pressure

8.5 Yield function in true stress space

From (70) and (77), yield function in the true stress space:

$$\hat{f}(\hat{\sigma}, \varepsilon_v^p) : \frac{(p - \pi_c)^2}{\pi_c^2} + \frac{q^2}{M^2 \pi_c^2} - 1 = 0 \quad (78)$$

8.6 Flow rule in true stress space

Yield function in the true stress space:

$$\hat{f}(\varepsilon_{ij}^p, \sigma_{ij}) = f(\varepsilon_{ij}^p, \frac{-\partial G}{\partial \varepsilon_{ij}^p}(\sigma_{ij}, \varepsilon_{ij}^p)) = 0 \quad (79)$$

Thus

$$\frac{\partial \hat{f}}{\partial \sigma_{ij}} = \frac{\partial f}{\partial \chi_{kl}} \frac{-\partial^2 G}{\partial \varepsilon_{kl}^p \partial \sigma_{ij}} \quad (80)$$

The flow rule now takes the form:

$$\Lambda \frac{\partial \hat{f}}{\partial \sigma_{ij}} = \Lambda \frac{\partial f}{\partial \chi_{kl}} \frac{-\partial^2 G}{\partial \varepsilon_{kl}^p \partial \sigma_{ij}} \quad (81)$$

$$\Lambda \frac{\partial \hat{f}}{\partial \sigma_{ij}} = \varepsilon_{ij}^p \quad (82)$$

As can be seen here, in Modified Cam Clay model, the flow rule is associated flow rule in true stress

9 Elastoplastic stiffness matrix Dep

The increment form of strain from (53)

$$\varepsilon_{ij} = -\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} \dot{\sigma}_{kl} - \frac{\partial^2 G}{\partial \sigma_{ij} \partial \varepsilon_{kl}^p} \dot{\varepsilon}_{kl}^p \quad (83)$$

Associated flow rule (82):

$$\dot{\varepsilon}_{kl}^p = \Lambda \frac{\partial \hat{f}}{\partial \sigma_{kl}} \quad (84)$$

From the yield function in eq(78), consistency condition is derived:

$$\dot{\hat{f}} = \frac{\partial \hat{f}}{\partial \sigma_{mn}} \dot{\sigma}_{mn} + \frac{\partial \hat{f}}{\partial \varepsilon_v^p} \dot{\varepsilon}_v^p = 0 \quad (85)$$

$$\dot{\hat{f}} = \frac{\partial \hat{f}}{\partial \sigma_{mn}} \dot{\sigma}_{mn} + \frac{\partial \hat{f}}{\partial \varepsilon_v^p} \Lambda \frac{\partial \hat{f}}{\partial \sigma_{mm}} \quad (86)$$

Thus, plastic multiplier is calculated as follow:

$$\Lambda = \frac{-\frac{\partial \hat{f}}{\partial \sigma_{mn}} \dot{\sigma}_{mn}}{\frac{\partial \hat{f}}{\partial \varepsilon_v^p} \frac{\partial \hat{f}}{\partial \sigma_{mm}}} \quad (87)$$

We substitute this into equation (53)

$$\varepsilon_{ij} = -\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} \dot{\sigma}_{kl} - \frac{\partial^2 G}{\partial \sigma_{ij} \partial \varepsilon_{kl}^p} \frac{\partial \hat{f}}{\partial \sigma_{kl}} - \frac{\frac{\partial \hat{f}}{\partial \sigma_{mn}} \dot{\sigma}_{mn}}{\frac{\partial \hat{f}}{\partial \varepsilon_v^p} \frac{\partial \hat{f}}{\partial \sigma_{mm}}} \quad (88)$$

$$\dot{\varepsilon}_{mn} = \left[-\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{mn}} + \frac{\frac{\partial^2 G}{\partial \sigma_{ij} \partial \varepsilon_{kl}^p} \frac{\partial \hat{f}}{\partial \sigma_{kl}}}{\frac{\partial \hat{f}}{\partial \varepsilon_v^p} \frac{\partial \hat{f}}{\partial \sigma_{mm}}} \right] \dot{\sigma}_{mn} \quad (89)$$

Thus, the Elastoplastic compliance matrix is :

$$C_{ep} = \left[-\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{mn}} + \frac{\frac{\partial^2 G}{\partial \sigma_{ij} \partial \varepsilon_{kl}^p} \frac{\partial \hat{f}}{\partial \sigma_{kl}}}{\frac{\partial \hat{f}}{\partial \varepsilon_v^p} \frac{\partial \hat{f}}{\partial \sigma_{mn}}} \right] \quad (90)$$

Note that the Elastic compliance matrix is :

$$C_e = \left[-\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{mn}} \right] \quad (91)$$

10 Derivative of G with respect to σ

10.1 $\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}}$

Set:

$$A = -\kappa p \left(\ln \frac{p}{p_R} - 1 \right) - \frac{q^2}{6g_s} \quad (92)$$

Notice that:

$$\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} = \frac{\partial^2 A}{\partial \sigma_{ij} \partial \sigma_{kl}} \quad (93)$$

$$\begin{aligned} \frac{\partial A}{\partial \sigma_{ij}} &= \frac{\partial A}{\partial p} \frac{\partial p}{\partial \sigma_{ij}} + \frac{\partial A}{\partial q} \frac{\partial q}{\partial \sigma_{ij}} \\ &= -\kappa \left[\ln \frac{p}{p_R} - 1 + p \frac{1}{p} \right] \frac{\delta_{ij}}{3} - \frac{q}{3g_s} \sqrt{\frac{3}{2}} \frac{S_{ij}}{\|S_{mn}\|} \\ &= -\frac{\kappa}{3} \delta_{ij} \ln \frac{p}{p_R} - \frac{q}{g_s \sqrt{6}} \frac{S_{ij}}{\|S_{mn}\|} = -\frac{\kappa}{3} \delta_{ij} \ln \frac{p}{p_R} - \frac{1}{2g_s} S_{ij} = B \\ \frac{\partial^2 A}{\partial \sigma_{ij} \partial \sigma_{kl}} &= \frac{\partial B}{\partial \sigma_{kl}} \\ &= \frac{\partial B}{\partial p} \frac{\partial p}{\partial \sigma_{kl}} + \frac{\partial B}{\partial q} \frac{\partial q}{\partial \sigma_{kl}} + \frac{\partial B}{\partial S_{ij}} \frac{\partial S_{ij}}{\partial \sigma_{kl}} \\ &= \left[-\frac{\kappa}{3} \delta_{ij} \frac{1}{p} \frac{\delta_{kl}}{3} \right] + 0 + \left[-\frac{1}{2g_s} \left(\delta_{ki} \delta_{lj} - \frac{1}{3} \delta_{ij} \delta_{kl} \right) \right] \\ &= -\frac{\kappa}{9p} \delta_{ij} \delta_{kl} - \frac{1}{2g_s} \left(\delta_{ki} \delta_{lj} - \frac{1}{3} \delta_{ij} \delta_{kl} \right) \end{aligned}$$

Finally:

$$\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} = -\frac{\kappa}{9p} \delta_{ij} \delta_{kl} - \frac{1}{2g_s} \left(\delta_{ki} \delta_{lj} - \frac{1}{3} \delta_{ij} \delta_{kl} \right) \quad (94)$$

It is worth to notice that $\partial^2 G / \partial \sigma_{ij} \partial \sigma_{kl}$ only depends on stress, not depend on strain Elastic compliance:

$$C_e = -\frac{\partial^2 G}{\partial \sigma_{ij} \partial \sigma_{kl}} = \frac{\kappa}{9p} \delta_{ij} \delta_{kl} + \frac{1}{2g_s} \left(\delta_{ki} \delta_{lj} - \frac{1}{3} \delta_{ij} \delta_{kl} \right) \quad (95)$$

$$10.2 \quad \frac{\partial^2 G}{\partial \sigma_{ij} \partial \varepsilon_{kl}^p}$$

$$\begin{aligned} \frac{\partial^2 G}{\partial \sigma_{ij} \partial \varepsilon_{kl}^p} &= -\frac{\partial(p\varepsilon_v^p + q\varepsilon_d^p)}{\partial \sigma_{ij} \partial \varepsilon_{kl}^p} \\ &= -\frac{\partial(\sigma_{ij}\varepsilon_{ij}^p)}{\partial \sigma_{ij} \partial \varepsilon_{kl}^p} \\ &= -\frac{\partial \varepsilon_{ij}^p}{\partial \varepsilon_{kl}^p} \\ &= -\delta_{ki}\delta_{lj} \end{aligned}$$

$$10.3 \quad \frac{\partial \hat{f}}{\partial \sigma_{mm}}$$

$$\frac{\partial \hat{f}}{\partial \sigma_{mm}} = \frac{\partial \hat{f}}{\partial p} \frac{\partial p}{\partial \sigma_{mm}} = \frac{2(p - \pi_c)}{\pi_c^2} \quad (96)$$

$$10.4 \quad \frac{\partial \hat{f}}{\partial \sigma_{mn}}$$

$$\begin{aligned} \frac{\partial \hat{f}}{\partial \sigma} &= \frac{\partial \hat{f}}{\partial p} \frac{\partial p}{\partial \sigma_{mn}} + \frac{\partial \hat{f}}{\partial q} \frac{\partial q}{\partial \sigma_{mn}} \\ &= \frac{2(p - \pi_c)}{\pi_c^2} \frac{\delta_{mn}}{3} + \frac{2q}{M^2 \pi_c^2} \frac{3S_{mn}}{2q} \\ &= \frac{2}{3} \frac{p - \pi_c}{\pi_c^2} \delta_{mn} + \frac{3}{M^2 \pi_c^2} S_{mn} \end{aligned}$$

$$10.5 \quad \frac{\partial \hat{f}}{\partial \varepsilon_v^p}$$

$$\begin{aligned} \frac{\partial \hat{f}}{\partial \varepsilon_v^p} &= \frac{\partial \hat{f}}{\partial \pi_c} \frac{\partial \pi_c}{\partial \varepsilon_v^p} \\ &= \left[-\frac{2p^2}{\pi_c^3} + \frac{2p}{\pi_c^2} - \frac{2q^2}{M^2 \pi_c^3} \right] \left[\frac{p_{c0}}{2} \frac{1}{\lambda - \kappa} \exp \frac{\varepsilon_v^p}{\lambda - \kappa} \right] \\ &= \left(-\frac{p^2}{\pi_c^3} + \frac{p}{\pi_c^2} - \frac{q^2}{M^2 \pi_c^3} \right) \frac{p_{c0}}{\lambda - \kappa} \exp \frac{\varepsilon_v^p}{\lambda - \kappa} \end{aligned}$$

11 Appendix

11.1 Find the equation for Gibbs energy

Rewrite the equation (20),(21) in case of triaxial tests

$$\varepsilon_v = -\frac{\partial G}{\partial p} = \varepsilon_v^e + \varepsilon_v^p \quad (97)$$

$$\varepsilon_d = -\frac{\partial G}{\partial q} = \varepsilon_d^e + \varepsilon_d^p \quad (98)$$

$$\chi_p = \pi = -\frac{\partial G}{\partial \varepsilon_v^p} = p - \rho \quad (99)$$

$$\chi_q = \tau = -\frac{\partial G}{\partial \varepsilon_d^p} = q \quad (100)$$

Relationships derive in the isotropic loading-unloading calculation:

- Elastic volumetric strain

$$\varepsilon_v^e = \kappa \ln \left(\frac{p}{p_R} \right) \quad (101)$$

- Elastic deviatoric strain: Assume the constant shear modulus

$$\varepsilon_d^e = \frac{q}{3g_s} \quad (102)$$

- Maximum preconsolidation pressure

$$p_{c0} = p_0 * \exp \frac{\left[\ln(1 + e_{NC}) - \lambda \ln \frac{p_0}{p_R} \right] - \ln(1 + e_0)}{\lambda - \kappa} \quad (103)$$

- Hardening rule

$$p_c = p_{c0} \exp \left(\frac{\varepsilon_v^p}{\lambda - \kappa} \right) \quad (104)$$

Finally, the Gibbs free energy equation is derived as follow:

$$G = -\kappa p \left(\ln \frac{p}{p_R} - 1 \right) - \frac{q^2}{6g_s} - (p\varepsilon_v^p + q\varepsilon_d^p) + \frac{1}{2}(\lambda - \kappa)p_{c0} \exp \left(\frac{\varepsilon_v^p}{\lambda - \kappa} \right) \quad (105)$$

11.2 Dissipative energy and plastic stored energy in Modified Cam Clay Model

11.2.1 Conventional Modified Cam Clay model

Yield surface:

$$f : q^2 - M^2 p(p_c - p) = 0 \quad (106)$$

Flow rule:

$$\dot{\varepsilon}_v^p = -\Lambda M^2 (p_c - 2p) \quad (107)$$

$$\dot{\varepsilon}_d^p = -2\Lambda q \quad (108)$$

11.2.2 Stress invariants in terms of ε^p and p_c

From (107),(108):

$$q = \frac{\dot{\varepsilon}_d^p}{2\Lambda}; p = \frac{1}{2} \left\{ p_c + \frac{\dot{\varepsilon}_v^p}{\Lambda M^2} \right\} \quad (109)$$

Insert into (106):

$$\left\{ \frac{\dot{\varepsilon}_d^p}{2\Lambda} \right\}^2 - M^2 \frac{1}{2} \left\{ p_c + \frac{\dot{\varepsilon}_v^p}{\Lambda M^2} \right\} \frac{1}{2} \left\{ p_c - \frac{\dot{\varepsilon}_v^p}{\Lambda M^2} \right\} = 0 \quad (110)$$

Solve the above equation to get:

$$\Lambda = \sqrt{\frac{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2}{M^2 p_c}} \quad (111)$$

$$p = \frac{1}{2} p_c + \frac{p_c \dot{\varepsilon}_v^p}{2\sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2}} \quad (112)$$

$$q = \frac{M^2 p_c \dot{\varepsilon}_d^p}{2\sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2}} \quad (113)$$

11.2.3 Plastic work increment

$$\dot{W}^p = p\dot{\varepsilon}_v^p + q\dot{\varepsilon}_d^p = \frac{1}{2}p_c\dot{\varepsilon}_v^p + \frac{1}{2}p_c\sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} \quad (114)$$

11.2.4 Dissipation energy function & Stored plastic energy function

From the first law of thermodynamics:

$$\dot{W}^p = \dot{F}^p + \dot{D} \quad (115)$$

And the equation (114), we can choose both dissipation energy function and stored plastic work energy based on the corresponding requirements:

- \dot{D} : Non-negative function. Its value equal zero when plastic strain occurs. And it necessarily be a homogeneous function of degree one with respect to plastic strain rate in case of rate-independent material. Therefore, it can be chosen as:

$$\dot{D} = \frac{1}{2}p_c\sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2} = \pi_c\sqrt{(\dot{\varepsilon}_v^p)^2 + M^2(\dot{\varepsilon}_d^p)^2}; \pi_c = \frac{p_c}{2} \quad (116)$$

- Stored plastic energy function: a state function
There is no strict sign requirement for F^p , it can be positive, negative or zero. But it should be integrable with respect to plastic strain. And for a close loop of plastic strain, the increment of this stored plastic energy function need to be zero. Hence, it can be chosen as:

$$\dot{F}^p = \frac{1}{2}p_c\dot{\varepsilon}_v^p = \frac{1}{2}p_c\dot{\varepsilon}_v^p \quad (117)$$

In Modified Cam Clay model, we choose:

$$F^p = \frac{1}{2}(\lambda - \kappa)p_R \exp \frac{\varepsilon_v^p}{\lambda - \kappa} \quad (118)$$

We can realize the relation between F^p and G^p :

$$F^p = G^p - (p\varepsilon_v^p + q\varepsilon_d^p) \quad (119)$$