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Review on Thermo-mechanical Approach in the Modelling of Geo-materials Incorporating Non- Associated Flow Rules

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Abstract

Recently, there has been a burgeoning interest in developing constitutive soil models from the laws of thermodynamics, mainly due to the benefits that these models automatically obey them and the approach provides a well-established structure and reduces the need for ‘ad hoc’ postulates. A thermodynamic framework, also known as thermo-mechanical framework, has the capability to predict the behaviour of geotechnical materials, which requires the anticipated incorporation of non-associated flow rules. As it is very challenging to achieve acceptable accuracy in plasticity modelling of granular materials, this paper aims to review this framework not only to discuss the details of the major components but also to highlight the capability of generating non-associated flow rules in a natural way from thermo-mechanical principles. This approach introduces the use of internal variables to develop the two thermodynamic potentials (the free energy and the rate of dissipation functions), sufficient to derive the corresponding yield function, flow rule, isotropic and kinematic hardening rules as well as the basic elasticity law. It is shown that the non-associated flow rule can be derived naturally from the postulated stress-dependent dissipation increment function. Comparison has been made with stress-independent dissipation to demonstrate that the approach can also successfully explain the behaviour of standard materials with associated flow rules. The basic steps for the thermo-mechanical formulation for developing a constitutive model are also reviewed and summarised. Furthermore, the power of conventional mathematical technique, Legendre transformation, in the derivation of constitutive equations has been highlighted.

Keywords: thermo-mechanical; free energy; dissipation; frozen elastic energy; geo-materials; granular.

1 Introduction

During the last decade, there has been a growing emphasis on the compliance of the developed constitutive soil models with the laws of thermodynamics, particularly the first and second laws. It was found out that the original Cam-clay model failed to invoke the second law of thermodynamics and hence, ultimately, led to its violation as a consequence. As a result, the modification of the Cam-clay model, i.e. modified Cam-clay model, abandoned the frictional mechanisms of energy dissipation in order to overcome the shortcomings of the original model and comply with the laws of thermodynamics. However, the modified Cam-clay model has not been able to incorporate non-associated flow rules, thus not capable to predict the behaviour of frictional geo-materials.

To be able to predict the behaviour of sands, rocks and other frictional geo-materials, it is now accepted that the constitutive modelling of such materials must include non-associated flow rules by formulating yield conditions and flow rules separately. Non-associated flow rules occur due to the interactions between the properties of frictional geo-materials.

Thermo-mechanical principles have been successfully applied to derive the yield condition and the flow rule from the dissipation function for the behaviour of standard materials with associated flow rules. However, non-associated flow rules can also be produced by following the thermo-mechanical approach, as suggested by (Collins & Houlsby, 1997). Therefore, a comprehensive review has been carried out to emphasise on the fact that if the dissipation function depends on the effective stress, as in the case of modelling dissipative geo-materials, non-associated flow rules can be generated automatically from thermo-mechanical principles. It is also discussed that the use of traditional mathematical procedure, termed “Legendre transformation”, plays a vital role in this approach.

2 Thermo-mechanical Framework

The most appropriate starting point for an isothermal deformation of materials can be written as:

$$\delta W = d\Psi + \delta\Phi, \text{ where } \delta\Phi \geq 0 \quad (1)$$

where δW is the incremental effective work done on a continuum element, $d\Psi$ is the differential of the free energy defined per unit volume and $\delta\Phi$ is the dissipation increment function defined per unit volume. $\delta\Phi$ must be non-negative in order to comply with the second law of thermodynamics. The free energy is a function of state variables, e.g. elastic and plastic strains. In contrast, Φ and W are not state functions. The free energy is assumed to be a function of total elastic strain tensor and plastic strain tensor, e_{ij} and e_{ij}^p , respectively. On the other hand, the dissipation function is assumed to depend additionally on plastic strain rate tensor, i.e., $\delta\Phi(e_{ij}, e_{ij}^p, de_{ij}^p)$. The validity of these assumptions can be found in (Collins & Houlsby, 1997) and (Collins & Kelly, 2002).

In general, the free energy is allowed to depend on both the elastic and plastic strains. This requires additional assumption, in which the material must be ‘decoupled’ in the sense that the instantaneous elastic moduli do not depend on the plastic strains. The special case comes from the above assumption that the free energy can be expressed as the sum of a function of only elastic strains, plus a function of only plastic strains. The validity of these assumptions can be found in (Collins & Houlsby, 1997) and (Collins & Kelly, 2002). From this ‘decoupled’ assumption, it follows that:

$$\Psi = \Psi^e(e_{ij}^e) + \Psi^p(e_v^p) \quad (2)$$

where Ψ^e and Ψ^p are the elastic and plastic components of the free energy function, e_{ij}^e is the elastic strain tensor and e_v^p is the plastic volumetric strain. (Ulm & Coussy, 2003) termed this as the ‘principle of separation of energies’. The additional term Ψ^p is the stored plastic work increment. This term is also coined as ‘frozen elastic energy’ in (Collins & Kelly, 2002). The storage of ‘frozen elastic energy’ is due to the inhomogeneous nature of the deformations at the micro scale. It is important to note the exclusion of plastic shear strain e_q^p from the plastic part of the free energy function. This is due to the assumption that plastic shear strains do not induce any ‘frozen elastic energy’, validated by the experimental findings, as confirmed in (Collins & Kelly, 2002).

Substituting (2) into (1) yields:

$$\delta W = d\Psi^e(e_{ij}^e) + d\Psi^p(e_v^p) + \delta\Phi \quad (3)$$

The total work increment can also be written as the sum of elastic and plastic components:

$$\delta W = \delta W^e + \delta W^p \quad (4)$$

From (3) and (4), it follows that:

$$\delta W^e = \sigma'_{ij} de_{ij}^e = \frac{\partial \Psi^e(e_{ij}^e)}{\partial e_{ij}^e} de_{ij}^e \quad \text{and} \quad \sigma'_{ij} = \frac{\partial \Psi^e(e_{ij}^e)}{\partial e_{ij}^e} \quad (5)$$

where, σ'_{ij} is the effective stress tensor. As we can see from the second part of (5), the basic elastic part of the constitutive law is deduced. Again, (3) and (4) provides:

$$\delta W^p = \sigma'_{ij} de_{ij}^p = d\Psi^p(e_v^p) + \delta\Phi(e_{ij}^p) = \frac{\partial \Psi^p(e_v^p)}{\partial e_v^p} de_v^p + \frac{\partial(\delta\Phi)}{\partial(de_{ij}^p)} de_{ij}^p \quad (6)$$

$$\delta W^p = \frac{\partial \Psi^p(e_v^p)}{\partial e_v^p} de_v^p + \frac{\partial(\delta\Phi)}{\partial(de_{ij}^p)} de_{ij}^p \quad (7)$$

Since $\delta\Phi$ is a homogeneous first order function of plastic strain rates de_{ij}^p , Euler’s theorem is used to obtain the last term in equation (6). Comparing with (7), this will only be satisfied if:

$$\rho'_{ij} = \frac{\partial \Psi^p(e_v^p)}{\partial e_v^p} \quad \text{and} \quad \chi_{ij} = \frac{\partial(\delta\Phi)}{\partial(de_{ij}^p)} \quad (8)$$

where, ρ'_{ij} and χ_{ij} are termed ‘shift’ stress and ‘dissipative’ stress respectively. This is supported by (Collins & Hilder, 2002) and (YangPing, WenJie, & NaiDong, 2013). However, (8) cannot be deduced formally as in the previous case of deducing elasticity law in (6). In order to achieve this, the status of a constitutive postulate termed as ‘Ziegler’s orthogonality postulate’ needs to be satisfied. The importance of this postulate can be found in (Houlsby & Puzrin, 2000) and (Collins & Houlsby, 1997). Referring to (7) and (8), it can be stated that the effective stress is the sum of the ‘shift’ stress and ‘dissipative’ stress and can be written as:

$$\sigma'_{ij} = \rho'_{ij} + \chi_{ij} \quad (9)$$

As a result, (6) can be rewritten as:

$$\delta W^p = \sigma'_{ij} de_{ij}^p = d\Psi_2 + \delta\Phi = \rho'_{ij} de_{ij}^p + \chi_{ij} de_{ij}^p \quad (10)$$

From (10), $\delta W^p = \sigma'_{ij} de_{ij}^p$; $d\Psi_2 = \rho'_{ij} de_{ij}^p$ and $\delta\Phi = \chi_{ij} de_{ij}^p$ can be deduced. Therefore, whilst the plastic work is the product of the true stress with the plastic strain increment, the plastic dissipation is the product of the dissipative stress with the plastic strain increment. In the conventional soil mechanics, the plastic work and the plastic dissipation are normally assumed to be equal. However, in the context of thermo-mechanics, these are only equal if the shift stress ρ'_{ij} is zero; in other words, the free energy is assumed to depend only on the elastic strains. In fact, this viewpoint is a cornerstone of modern soil mechanics. The importance of the shift stress in the modelling of the unloading situations can be found in (Collins & Kelly, 2002) and (Collins, Bai, & Siyin, 2007). Moreover, (Collins & Kelly, 2002) recognised the importance of this ‘stored plastic work’ as they discussed the concept in terms of both the thermo-mechanical and the micromechanical viewpoints.

3 Relationship between Dissipation Function and Yield Function

The other major step of the thermo-mechanical approach is to specify the dissipation increment function to derive the whole constitutive formulation. The study of the isothermal deformations of different types of material can be carried out by postulating different functional forms for $\delta\Phi$. These can be found as examples in the books by (Ziegler, 1983) and (Maugin, 1992).

3.1 Stress-Dependent Dissipation Function for the Modelling of Dissipative Materials

For the modelling of dissipative geo-materials, the dissipation increment function must take the form $\delta\Phi(\sigma'_{ij}, e_{ij}^p, de_{ij}^p)$ instead of $\delta\Phi(e_{ij}^p, de_{ij}^p)$ to take into account of current stress level. Please note here that $\delta\Phi$ cannot depend on the total strain increments as this could mean a purely elastic deformation would produce dissipation. Since $\delta\Phi$ must have the dimensions of (stress)(time)⁻¹, (Collins & Houlsby, 1997) suggested the following conditions:

- In the case of frictional materials, the dissipation increment function must include one or more of the stress components explicitly, or
- In the critical state models, it must contain a function, which has the dimension of stress, i.e. being related to the normal pre-consolidation pressure.

If a material is to exhibit rate-independent behaviour, then $\delta\Phi$ must be a homogeneous first order function of strain rates, de_{ij}^p . Hence, the partial derivative of the dissipation increment function with respect to the plastic strain rate, de_{ij}^p , can then be obtained as follows:

$$\chi_{ij} = \frac{\delta\Phi(\sigma'_{ij}, e_{ij}^p, de_{ij}^p)}{\partial (de_{ij}^p)} \quad (11)$$

Here, the σ'_{ij} term in the modified dissipation increment function are treated as independent constant parameters while obtaining derivatives and χ_{ij} is the “dissipative” stress tensor. As there are both volumetric and shear components, “tensor” symbol is used here for simplification. Then, a Legendre transformation is performed on $\delta\Phi(\sigma'_{ij}, e_{ij}^p, de_{ij}^p)$ to introduce its Legendre dual function, $f(\sigma'_{ij}, e_{ij}^p, \chi_{ij})$ say, with the main property that:

$$\delta\Phi(\sigma'_{ij}, e_{ij}^p, de_{ij}^p) + f(\sigma'_{ij}, e_{ij}^p, \chi_{ij}) = \chi_{ij} de_{ij}^p \quad (12)$$

Since $\delta\Phi$ is a homogeneous first order function of strain rates, the Legendre transformation is singular. Details of singular Legendre transformation is discussed in the (Collins, 1997) and (Collins & Houslyby, 1997), where it is demonstrated that the Legendre dual of a homogeneous first order function is identically zero. Therefore, it follows from (12) that:

$$f(\sigma'_{ij}, e_{ij}^p, \chi_{ij}) = 0 \quad (13)$$

Since the transformation is singular, the dual relation to (12) is not unique – see (Collins, 1997) and (Collins & Houslyby, 1997). Therefore, the time derivatives of the internal parameters are provided by:

$$de_{ij}^p = \lambda \frac{\partial f(\sigma'_{ij}, e_{ij}^p, \chi_{ij})}{\partial \chi_{ij}} \quad (14)$$

The dual relationships for the passive variables provided by Legendre transformation is given by:

$$\frac{\delta\Phi(\sigma'_{ij}, e_{ij}^p, de_{ij}^p)}{\partial \sigma'_{ij}} = -\lambda \frac{\partial f(\sigma'_{ij}, e_{ij}^p, \chi_{ij})}{\partial \sigma'_{ij}} \quad \text{and} \quad \frac{\delta\Phi(\sigma'_{ij}, e_{ij}^p, de_{ij}^p)}{\partial e_{ij}^p} = -\lambda \frac{\partial f(\sigma'_{ij}, e_{ij}^p, \chi_{ij})}{\partial e_{ij}^p} \quad (15)$$

where, λ is an undetermined multiplier. Equation (13) represents none other than the yield condition, whereas (14) is the associated or normal flow rule in the conventional plasticity. As a result, the yield function can be derived automatically from the postulate of a rate-independent dissipation function. However, both of these equations are expressed in the dissipative stress space not the actual stress space. The proof of this outcome has also been provided by (Houslyby, 1981).

Since the yield condition and the associated flow rule are expressed in the dissipative stress space f , these expressions are required to be transformed to the actual stress space. In order to do so, it is required to replace χ_{ij} in (13) by σ_{ij} . Then, this can easily be achieved by using ‘decoupled’ assumption, i.e. by re-arranging (9). Therefore, the yield function in actual stress space, $\bar{f}(\sigma'_{ij}, e_{ij}^p)$, can then be defined as follows:

$$\bar{f}(\sigma'_{ij}, e_{ij}^p) = f(\sigma'_{ij}, e_{ij}^p, \chi_{ij}) = f(\sigma'_{ij}, e_{ij}^p, \sigma'_{ij} - \rho'_{ij}) = 0 \quad (16)$$

Differentiate (16) with respect to the stress components, i.e. actual and dissipative stress components:

$$\frac{\partial \bar{f}}{\partial \sigma'_{ij}} = \frac{\partial f}{\partial \sigma'_{ij}} + \frac{\partial f}{\partial \chi_{ij}} \quad (17)$$

Using (14) and (15), it follows that:

$$de_{ij}^p = \lambda \frac{\partial \bar{f}}{\partial \sigma'_{ij}} + \frac{\delta \Phi}{\partial \sigma'_{ij}} \tag{18}$$

From (18), the flow rule becomes non-associated in the actual stress space, as $\delta\Phi$ depends explicitly on effective stress. If the dissipation increment function does not depend on the effective stress, the last term in (18) can then be ignored, thus retaining the associated flow rule in both dissipative and actual stress planes. Equations (12) – (18) indicate that this non-associated flow rule is derived naturally from the general thermo-mechanical framework, using stress-dependent $\delta\Phi$ function. It is demonstrated that no new function needs to be introduced and no new hypothesis has to be postulated in order to derive the constitutive equations for predicting the behaviour of geo-materials.

4 Thermo-mechanical Formulation

In this paper, the basic steps in developing an elastic/plastic model for geo-materials using thermo-mechanical approach are also reviewed and can be summarised, as shown in Figure 1 and Table 1.

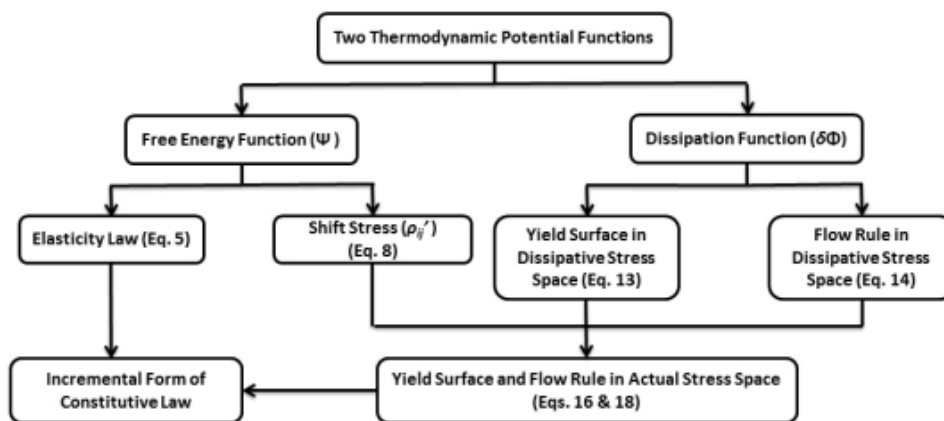


Figure 1: Flow chart in constructing the incremental form of the elastic/plastic constitutive law, starting with the free energy and dissipation functions (Modified from (Collins & Kelly, 2002))

From this review, the primary benefits are summarised as follows:

1. All the constitutive models developed within this framework automatically obey thermodynamic laws.
2. The framework makes considerable use of potential functions.
3. The theory has a well-defined structure and reduces the need for ‘ad hoc’ assumptions.
4. The approach allows a number of competing models to be developed within this core framework, and hence, allow them to be comfortably compared to determine advantages and drawbacks easily and effectively.
5. The theory is adequately flexible to incorporate the attributes for predicting friction and dilation, particularly crucial in modeling granular geo-materials with acceptable accuracy.

| | |
|--|---|
| Free Energy Function | $\Psi = \Psi(\sigma_{ij}, e_{ij}^e, e_v^p)$ |
| Stress Tensor | $\sigma'_{ij} = \frac{\partial \Psi^e(e_{ij}^e)}{\partial e_{ij}^e}$ |
| Shift Stress Tensor | $\rho'_{ij} = \frac{\partial \Psi^p(e_v^p)}{\partial e_v^p}$ |
| Dissipative Stress Tensor | $\chi_{ij} = \frac{\partial(\delta\Phi)}{\partial(de_{ij}^p)}$ |
| Dissipation Function | $\delta\Phi(\sigma'_{ij}, e_{ij}^p, de_{ij}^p) \geq 0$ |
| Yield function in the dissipative stress space | $f(\sigma'_{ij}, e_{ij}^p, \chi_{ij}) = 0$ |
| Yield function in the actual stress space | $\bar{f}(\sigma'_{ij}, e_{ij}^p) = 0$ |
| Non-associated flow rule | $de_{ij}^p = \lambda \frac{\partial \bar{f}}{\partial \sigma'_{ij}} + \frac{\delta\Phi}{\partial \sigma'_{ij}}$ |

Table 1: Basic Formulations for Thermo-mechanical Framework

Central to this thermo-mechanical approach is the recognition that not all the plastic work during irreversible deformation is dissipated. Some portion of this work is, in general, being stored. Although it has been recognised in the literature associated with metals, it is still left to be fully appreciated and applied in the geo-mechanics context. However, there were some papers discussed by (Palmer, 1967), who demonstrated that part of the plastic work in the classical critical state models is stored; (Houlsby, 1981) also highlighted this fact in his Ph.D Thesis and tried to revisit the early Cambridge models using thermo-mechanics; and (Jefferies, 1993) asserted the argument that a quarter of the plastic work is stored in his Nor-sand model. Therefore, it is acknowledged that further studies would be required to evaluate the thermodynamic consistency of recent constitutive models modelling time-dependent behaviour of soft clays, cemented soils and unsaturated soils for practical purposes (e.g. Nguyen et al., 2014; Le et al., 2015; Ho et al., 2015,2016).

5 Conclusion

In this paper, a thermo-mechanical framework for plasticity formulation is reviewed primarily for the development of constitutive models for predicting the behaviour of granular geo-materials. As this is an on-going research, the major purpose is to prepare a comprehensive thermo-mechanical framework for the development of constitutive soil models, which are important in achieving the versatility and the capability to predict behaviour of different types of geo-materials. Using thermo-mechanical framework, it is shown that constructing plasticity models from the two major potentials (free energy and dissipation increment functions) requires a two-stage process; firstly, the yield condition and the flow rule being constructed in the dissipative stress space, and then transferred to actual stress space in the latter stage. This review proves to be very valuable as it provides detailed steps with much clarification, revealing the important relationships between the dissipation increment function, the yield surface and the flow rule. The yield surface and the non-associated behaviour of the flow rule seem to be a necessary consequence of the proposed dissipation function and are seen to be intimately connected. Most importantly, it is well documented that the framework allows the incorporation of non-associated flow rules into the elastic/plastic constitutive models without violating

any thermodynamic laws. This paper also reveals the power of conventional mathematical approach, i.e. Legendre transformation, in deriving constitutive equations effectively and efficiently.

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