

A Generalized Thermomechanic Approach

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ABSTRACT

A generalized thermomechanic approach is obtained starting with an analysis of internal variables and thermodynamic potentials dealing with classical thermodynamics. This concept is extended for small deformations in continuum mechanics, where after applying conservation of mass, balance of linear momentum, balance of moment of momentum, the first and second law of thermodynamics the Clausius-Duhem inequality is obtained. After applying the normality rule and making use of Lagrange multipliers and yield functions it was concluded for n-state equations (for n-state variables) m-yield functions ($m \leq n$) are used to define the internal state variables evolution.

Keywords: Thermomechanics, Lagrange multipliers, Clausius-Duhem, Normality rule

1. CLASSICAL THERMODYNAMICS

Thermodynamics deals with systems which are at rest from a phenomenological or macroscopic point of view. Let the state of such a system be described by a set of mutually independent *kinematic variables, coordinates, or parameters* $a^{(k)}$ ($k = 0, 1, \dots, n$) (Coleman and Gurtin, 1967, Germain *et al*, 1983, and Ziegler, 1983). The parameter $a^{(k)}$ could be a scalar, vector, tensor, or function as defined by the problem to be analyzed.

The *first fundamental law of thermodynamics*, often called the law of conservation of energy, states that there is a state function called internal energy, defined in terms of the kinematic variables $U(a^{(0)}, a^{(1)}, \dots, a^{(n)})$, for a closed system, is $dU = \delta Q + \delta W$; where dU is total differential increase of the internal energy of the system, δQ is an infinitesimal amount of heat supplied to the system, and δW is the infinitesimal elementary work done on the system. The use of δ denotes an inexact differential, i.e., there is no function Q or W that can be differentiated to yield δQ or δW .

The term state function is commonly defined as a property of the system that depends on the current state, that is dependent of the mutually independent kinematic variables $\{a^{(0)}, a^{(1)}, \dots, a^{(n)}\}$. This state function is path-independent or not dependent on the way the system has reached the current state and describes quantitatively the equilibrium state of thermodynamic systems. Also it should be pointed out that state functions are extensive quantities (i.e., a physical quantity whose values are proportional to the size of the system it describes).

Rudolf Clausius formulated in 1865 the *second fundamental law of thermodynamics* and coined the term entropy (from the Greek *entropē*, change). He stated that entropy, a measure of the amount of energy which is unavailable to do work, of any isolated thermodynamic system tends to increase over time, approaching a maximum value.

Entropy is an extensive state function, whose change between two equilibrium states dS could be determined quantitatively by the transferred reversible heat δQ and the absolute temperature θ , as $dS = \delta Q/\theta$.

When a mechanical system is considered, a small increment in energy or mechanical work is the product of a force times a small displacement, when both are measured in the same direction. An extension of this concept is applied to thermodynamics, so an increment in the total change of energy or work can be expressed as the sum of the products of certain *generalized forces* $A^{(k)}$, and their corresponding small *generalized displacements* $a^{(k)}$. Each pair of generalized force and associated displacement is called *conjugate variables*, where intensive and extensive quantities are considered for generalized forces and displacements correspondingly. Then the infinitesimal elementary work done on the system is of the form $\delta W = A^{(k)} da^{(k)}$, wherein the summation convention is implied. All work functions are path-dependent, so from the thermodynamics point of view they are not state functions. It is a matter of experience when various work effects should be taken into account. In some cases their contribution may be so small as to be neglected.

Maugin,1999, expresses the Corollary of Carnot's theorem where a thermodynamic system can always be described by the state variables $\{a^{(0)} = S, a^{(1)}, \dots, a^{(n)}\}$ in such a way that the first and second thermodynamic laws are considered. Then the internal energy is a function of the kinematic variables $U(S, a^{(1)}, \dots, a^{(n)})$, so when the differential is performed the following relation is obtained

$$dU = \frac{\partial U}{\partial S} dS + \sum_{k=1}^n \frac{\partial U}{\partial a^{(k)}} da^{(k)} \quad (1)$$

After substituting previously defined relations into Equation 1, we get

$$dU = \theta dS + \sum_{k=1}^n A^{(k)} da^{(k)} \quad (2)$$

The comparison of Eqs. (3.4) and (3.5) gives Equation (3). in such a manner that θ and $A^{(k)}$ are positively homogeneous functions of degree zero, with both as intensive variables of state.

$$\theta = \frac{\partial U}{\partial S} dS, \quad A^{(k)} = \frac{\partial U}{\partial a^{(k)}}, \quad k = 1, 2, \dots, n \quad (3)$$

2. INTERNAL STATE VARIABLES

2.1 CLASSICAL THERMODYNAMICS

Classical thermodynamics makes use of four basic quantities, two intensive variables (pressure and temperature) and two extensive variables (volume and entropy). Temperature and entropy are considered conjugate variables as defined earlier. In classical thermodynamics, pressure and volume are also conjugate variables.

Four quantities called thermodynamic potentials are well defined state functions and used in the classical thermodynamics to characterize various macroscopic systems. They are the internal energy u , Helmholtz free energy ψ , enthalpy h , and Gibbs free energy g , with all four having units of energy. All four are related through the Legendre transformation, which, for a general case, describes a convex function using a different set of variables, namely the gradients of the original function. Several authors (Houlsby and Puzrin ,2000, Gelfand and Fomin,1963, and Maugin and Morro,1989) defined this transformation. So, given the function $A(x^{(1)}, \dots, x^{(m)}; \alpha^{(1)}, \dots, \alpha^{(n)})$ it can be transformed to its dual function $B(x^{(1)}, \dots, x^{(m)}; \beta^{(1)}, \dots, \beta^{(n)})$ using

$$B(x^{(1)}, \dots, x^{(m)}; \beta^{(1)}, \dots, \beta^{(n)}) = \min \left(\pm A(x^{(1)}, \dots, x^{(m)}; \alpha^{(1)}, \dots, \alpha^{(n)}) \mp \sum_{k=1}^n \alpha^{(k)} \beta^{(k)} \right) \quad (4)$$

where, $\beta^{(k)} = \frac{\partial A}{\partial \alpha^{(k)}}$, $\alpha^{(k)} = \mp \frac{\partial B}{\partial \beta^{(k)}}$, $X^{(i)} = \frac{\partial A}{\partial x^{(i)}} = \pm \frac{\partial B}{\partial x^{(i)}}$ for $k = 1, 2, \dots, n$; $i = 1, 2, \dots, m$

The variables $x^{(i)}$ play a passive role in this transformation and are treated as constant parameters. In the case of thermodynamics the variables $\alpha^{(k)}$ and $\beta^{(k)}$ are conjugate variables, as $x^{(i)}$ and $X^{(i)}$. The use of this dual function provides the most convenient description of the system in study, i.e., the one that best determines the stability of a system and how the system evolves towards equilibrium.

Table 1: Thermodynamic Potentials in Classical Thermodynamics

	Internal energy	Helmholtz free energy	Enthalpy	Gibbs free energy
<i>Natural variables</i>	$U = U(V, S)$	$\Psi = \Psi(V, \theta)$ $\Psi = U - S\theta$	$H = H(p, S)$ $H = U + pV$	$Z = Z(p, \theta)$ $Z = H - S\theta = \Psi + pV$
	$p = -\frac{\partial U}{\partial V}$ $\theta = \frac{\partial U}{\partial S}$	$p = -\frac{\partial \Psi}{\partial V}$ $S = -\frac{\partial \Psi}{\partial \theta}$	$V = \frac{\partial H}{\partial p}$ $\theta = \frac{\partial H}{\partial S}$	$V = \frac{\partial Z}{\partial p}$ $S = -\frac{\partial Z}{\partial \theta}$

The thermodynamic potentials in classical thermodynamics are expressed as functions of so-called natural variables, as expressed in Table 1. When the differential work equation for pressure and volume is taken as $-p dV$, as expressed in Table 1, Maxwell's relations arise from further partial differentiation of expressions in the last row of Table 1; they can also be defined using a Legendre theorem as expressed above.

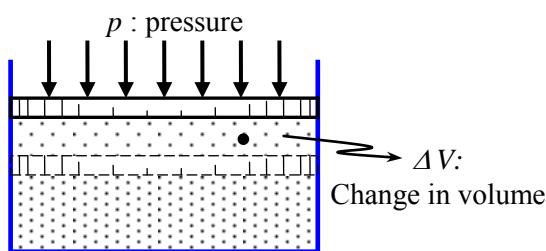


Figure 1: Ideal Gas inside a Cylinder

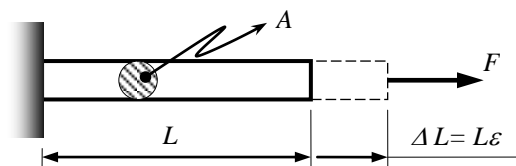


Figure 2: Bar Under Tension

For an ideal gas, considering a homogeneous, quasi-static, and reversible closed system process, the elementary work done when a pressure produces a change in volume (neglecting all other electrical, chemical, etc. processes) is defined as $\delta W = -p dV$ (see Figure 1). After the second thermodynamic law and this definition are applied to the first thermodynamic law, the differential internal energy can then be defined as $dU = -pdV + \theta ds$. When divided by its mass, the specific internal energy is derived as $du = -pdv + \theta ds$. For the specific internal energy defined as a function of the specific volume and the specific entropy, $u(v, s)$, its derivative could be found using the chain rule as:

$$du(v, s) = \frac{\partial u}{\partial v} dv + \frac{\partial u}{\partial s} ds \quad (4)$$

2.2 UNIAXIAL STRAINS

It has been seen previously that the increase in the internal energy is related to the pressure and change in volume. In the case of solids, this relation is between stress and the change in strain and known as *strain energy*.

An elemental definition of the strain energy is that it is the increase in energy associated with the deformation of a bar subjected to a tensile force, Beer et al., 2006. For the case of a bar under tension, Figure 3-2, the elementary work is equal to the load F times a small (differential) change in the elongation $d(L\varepsilon)$, or $\delta W = -F d(L\varepsilon)$.

Following the same procedure as in the case of ideal gases and applying the conditions for differential change in the elongation, the specific internal energy is then found to be $du = \sigma d\varepsilon/\rho + \theta ds$. When the specific internal

energy is defined as a function of the specific variables volume and entropy, $u(\varepsilon, s)$, it follows that its Legendre relations are

$$\sigma = \rho \frac{\partial u(\varepsilon, s)}{\partial \varepsilon} ; \theta = \frac{\partial u(\varepsilon, s)}{\partial s} \quad (5)$$

2.3 SMALL DEFORMATIONS IN CONTINUUM MECHANICS

A more general case must consider the balance of some physical quantities. These balance laws are related to the conservation of mass, linear momentum and angular momentum, balance of energy, and entropy generation. The balances are defined initially in the context of global relationships and develop into field equations (Chadwick, 1976; Spencer, 1983; Marsden and Hughes, 1983; Mase and Mase, 1999; and Reddy, 2002).

In order to obtain these field equations from its balance law, certain considerations must be taken. Only small deformations are to be considered from here on, so current, spatial, or Eulerian configuration is to be used. That is, the Lagrange finite strain tensor and the Eulerian strain tensor are assumed the same and equal to a single infinitesimal strain tensor ε_{ij} , defined as $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$.

The physical quantities under consideration are those that act over the continuum, some over the surface dS (defined by its normal n_i) and others through the volume dV , as seen in Figure 3. The mechanical effects are the internal forces per unit mass b_i and the surface tractions $t_i^{(n)}$, that act over the volume and surface respectively.

The heat supply, per unit mass r is produced by internal sources which act through the volume; while the heat flux per unit area and per unit time q_i conducted into the body act over the surface when thermal effects are considered. The density of the continuum ρ is also considered and defined through the volume and per unit volume. It will be considered that all quantities are function of time and position (t, x_i) and constant over the differential element.

Conservation of mass: The mass of the body remains constant in time, invariant under motion, regardless of the used configuration, so

$$m = \frac{d}{dt} \int_V \rho dV = 0 \Rightarrow \rho + \rho v_{i,i} = 0 \quad (\text{Continuity equation}) \quad (6)$$

Balance of linear momentum: The rate of change of the linear momentum equals the net force (surface and body forces) exerted over the body, so

$$\frac{d}{dt} \int_V \rho v_i dV = \int_V \rho b_i dV + \oint_S \rho t_i^{(n)} dS \Rightarrow \sigma_{ji,j} + \rho b_i = \rho \dot{v}_i \quad (\text{Equation of motion}) \quad (7)$$

Balance of moment of momentum: The rate of change of the moment of momentum with respect to any given point equals the moment exerted by the surface and body forces with respect the same point, then

$$\frac{d}{dt} \int_V \varepsilon_{ijk} x_j \rho v_k dV = \int_V \varepsilon_{ijk} x_j \rho b_k dV + \oint_S \varepsilon_{ijk} x_j \rho t_k^{(n)} dS \Rightarrow \sigma_{ij} = \sigma_{ji} \quad (8)$$

First law of thermodynamics: For this effect, a balance of energy is performed for only mechanical and thermal considerations, not including electrical, chemical, magnetic, or other energies. So, the change of total energy of a material region or the sum of rates of the specific internal energy and specific kinetic energy is equal to the sum of rates of work power of the mechanical power and thermal energy.

$$\frac{d}{dt} \int_V \rho \left(u + \frac{1}{2} v_i v_i \right) dV = \int_V \rho (b_i v_i + r) dV + \oint_S \rho (t_i^{(n)} v_i - q_i n_i) dS \Rightarrow \rho \dot{u} - \sigma_{ij} \varepsilon_{ij} - \rho r + q_{i,i} = 0 \quad (\text{Energy equation}) \quad (9)$$

The rate of work is due to the internal forces per unit mass b_i and the surface tractions $t_i^{(n)}$, right side of Equation (9). The heat supply per unit mass r produced by internal sources and the heat flux per unit area and per unit time q_i conducted into the body are acting over the volume and surface respectively, defining the rate of thermal energy. These effects of mechanical and thermal sources can be observed in Figure 3.

Second law of thermodynamics: The rate of change of entropy or entropy production is equal or bigger than the change in entropy due to the heat produced by internal sources and flux entering the continuum over its absolute temperature, then

$$\frac{d}{dt} \int_V \rho s dV \geq \int_V \frac{\rho r}{\theta} dV - \int_S \rho \frac{q_i n_i}{\theta} dS \Rightarrow \rho \theta \dot{s} - \rho r + q_{i,i} - q_i \frac{\theta_{,i}}{\theta} \geq 0 \quad (\text{Clausius-Duhem equation}) \quad (10)$$

Collins and Housby, 1997, Housby and Puzrin, 2000, and Basaran and Nie, 2004, observed a dissipation process from the Clausius-Duhem equation, Equation 10, whenever an irreversible process is taken into account. Additionally, since each dissipation must be greater than zero, then it is widely accepted that each dissipation component must be also non-negative, or

$$\rho \theta \dot{s} - \rho r + q_{i,i} \geq 0; \quad -q_i \frac{\theta_{,i}}{\theta} \geq 0 \quad (11)$$

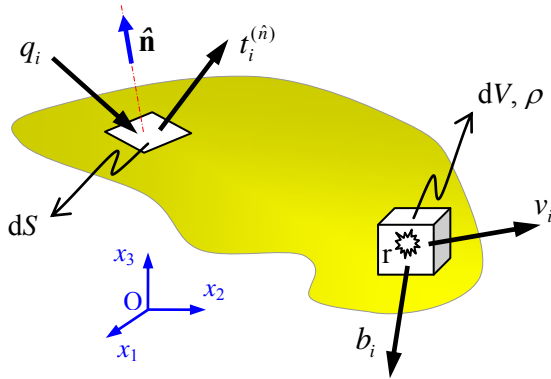


Figure 3: Mechanical and Thermal Effects Over a Continuum

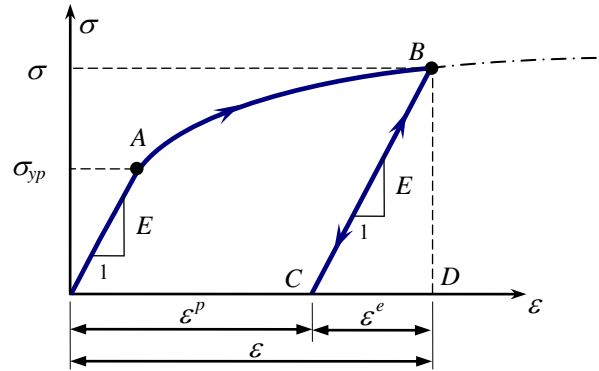


Figure 4: Additive Strain Decomposition for Small Deformations

When a reversible process is taken into account, no dissipation is expected. Then, the dissipation observed in Equation 11 should be zero, and employing the definition of the rate of internal energy, then

$$\dot{u} = \frac{\sigma_{ij}}{\rho} \dot{\epsilon}_{ij} + \theta \dot{s} \quad (12)$$

So, when the internal energy is defined with respect to the internal state variables, strain, and entropy, $u(\epsilon, s)$, then its derivative is stated in Equation 13 and its Legendre relations are defined as seen in Table 2.

$$du(\epsilon_{ij}, s) = \frac{\partial u}{\partial \epsilon_{ij}} d\epsilon_{ij} + \frac{\partial u}{\partial s} ds \quad (13)$$

Table 2: Specific Thermodynamic Potentials for Small Deformations

Internal energy	Helmholtz free energy	Enthalpy	Gibbs free energy
$u = u(\epsilon_{ij}, s)$	$\psi = \psi(\epsilon_{ij}, \theta) = u - s\theta$	$h = h(\sigma_{ij}, s) = u - \sigma_{ij}\epsilon_{ij}$	$\zeta = \zeta(\sigma_{ij}, \theta) = h - s\theta = \psi - \sigma_{ij}\epsilon_{ij}$
$\sigma_{ij} = \rho \frac{\partial u}{\partial \epsilon_{ij}}; \theta = \frac{\partial u}{\partial s}$	$\sigma_{ij} = \rho \frac{\partial \psi}{\partial \epsilon_{ij}}; s = -\frac{\partial \psi}{\partial \theta}$	$\epsilon_{ij} = \rho \frac{\partial h}{\partial \sigma_{ij}}; \theta = \frac{\partial h}{\partial s}$	$\epsilon_{ij} = \rho \frac{\partial \zeta}{\partial \sigma_{ij}}; s = -\frac{\partial \zeta}{\partial \theta}$

2.4 GENERALIZED STATE VARIABLES FOR SMALL DEFORMATIONS IN CONTINUUM MECHANICS

The similarities between the models presented until this point are obvious. The equations of state, that associate thermodynamic forces to the derivative of the potential with respect to its natural variables, for the temperature is the same for the cases of classical thermodynamics, uniaxial loading, and small deformation in continuum mechanics. This is also seen when pressure is expressed as the negative of the derivative of the internal energy

w.r.t. the volume, or the specific volume when the specific internal energy is considered, when compared to the stress. This relation could be seen also when the pressure is stated as a mean normal stress, $p = -\sigma_{ii}/3$, and the change in volume or cubic dilatation as the first invariant of the strain, $\Delta V/V = \varepsilon_{ii}$.

Also, it should be noted that strain seen until now is the elastic strain. No assumption has been made until now about the total strain having some elastic and plastic components. So, an additive decomposition of this elastic strain, as seen in Figure 2, is defined as $\varepsilon_{ij}^e = \varepsilon_{ij} - \varepsilon_{ij}^p$.

For a general case, the specific internal energy is defined as a function of the elastic strain, specific entropy, and several internal variables, $u(\varepsilon_{ij}^e, s, a^{(k)})$, where an extension of the previous concepts are employed in order to include some generalized state variables. First, the additive decomposition of strain is considered, this is done in order to define the internal energy as a function of the total strain. So from the additive decomposition of strains, the elastic strain is set to be function of the total and plastic strain, then the internal energy would be a function of both, as $u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})$, and its equations of state are then reformulated considering,

$$\frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial \varepsilon_{ij}} = \frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial (\varepsilon_{ij} - \varepsilon_{ij}^p)} \cdot \frac{\partial (\varepsilon_{ij} - \varepsilon_{ij}^p)}{\partial \varepsilon_{ij}} = \frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial (\varepsilon_{ij} - \varepsilon_{ij}^p)} \cdot \mathbf{I} = \frac{\partial u(\varepsilon_{ij}^e, s, a^{(k)})}{\partial \varepsilon_{ij}^e} = \frac{\sigma_{ij}}{\rho}$$

and

$$\frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial \varepsilon_{ij}^p} = \frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial (\varepsilon_{ij} - \varepsilon_{ij}^p)} \cdot \frac{\partial (\varepsilon_{ij} - \varepsilon_{ij}^p)}{\partial \varepsilon_{ij}^p} = \frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial (\varepsilon_{ij} - \varepsilon_{ij}^p)} \cdot (-\mathbf{I}) = -\frac{\partial u(\varepsilon_{ij}^e, s, a^{(k)})}{\partial \varepsilon_{ij}^e} = -\frac{\sigma_{ij}}{\rho}$$

so, when its derivative is obtained as

$$du(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)}) = \frac{\partial u}{\partial \varepsilon_{ij}} d\varepsilon_{ij} + \frac{\partial u}{\partial \varepsilon_{ij}^p} d\varepsilon_{ij}^p + \frac{\partial u}{\partial s} ds + \sum_{k=1}^n \frac{\partial u}{\partial a^{(k)}} da^{(k)} = \frac{\partial u}{\partial \varepsilon_{ij}^e} d\varepsilon_{ij}^e + \frac{\partial u}{\partial s} ds + \sum_{k=1}^n \frac{\partial u}{\partial a^{(k)}} da^{(k)}$$

then it can be seen that the derivative of the internal energy is function of the elastic strain:

$$\sigma_{ij} = \rho \frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial \varepsilon_{ij}^e}; \theta = \frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial s}; A^{(k)} = -\rho \frac{\partial u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})}{\partial a^{(k)}} \quad (14)$$

The thermodynamic forces $A^{(k)}$ are taken as the negative of the density, times the partial derivative of its internal variable $a^{(k)}$ by extension from the previous exposed concepts. The nature of this equation of state is explained in detail when a dissipation phenomenon is analyzed. Based on the equations of state defined in Equation 14, Table 3 is completed without considering the enthalpy potential as it does not have physical meaning when continuum mechanics is considered.

Table 3: Specific Thermodynamic Potentials for Small Deformations in Continuum Mechanics

Internal energy	Helmholtz free energy	Gibbs free energy
$u = u(\varepsilon_{ij}, \varepsilon_{ij}^p, s, a^{(k)})$	$\psi = \psi(\varepsilon_{ij}, \varepsilon_{ij}^p, \theta, a^{(k)}) = u - s\theta$	$\zeta = \zeta(\sigma_{ij}, \theta, a^{(k)}) = \psi - \sigma_{ij}\varepsilon_{ij}^e$
$\sigma_{ij} = \rho \frac{\partial u}{\partial \varepsilon_{ij}^e}; \theta = \frac{\partial u}{\partial s}$	$\sigma_{ij} = \rho \frac{\partial \psi}{\partial \varepsilon_{ij}^e}; s = -\frac{\partial \psi}{\partial \theta}$	$\varepsilon_{ij}^e = -\rho \frac{\partial \zeta}{\partial \sigma_{ij}}; s = -\frac{\partial \zeta}{\partial \theta}$
$A^{(k)} = -\rho \frac{\partial u}{\partial a^{(k)}}$	$A^{(k)} = -\rho \frac{\partial \psi}{\partial a^{(k)}}$	$A^{(k)} = -\rho \frac{\partial \zeta}{\partial a^{(k)}}$

3. ENTROPY GENERATION

A model is better defined using the specific Helmholtz free energy as the thermodynamic potential than the internal energy because it is difficult to use the entropy as a state variable; though using the temperature is more suitable. So, taking the time derivative of the Helmholtz free energy when it is defined as a function of the

internal energy, or $\psi = u - s\theta - s\theta$ and substituting the definitions made previously for the first and second law of thermodynamics, the Clausius-Duhem inequality becomes,

$$\sigma_{ij} \dot{\varepsilon}_{ij} - \rho(\dot{\psi} + s\dot{\theta}) - q_i \frac{\theta_{,i}}{\theta} \geq 0 \quad (15)$$

As considered initially, the total strain is the addition of the elastic and plastic strains. Thus, the total strain rate is also the addition of the time derivatives of the plastic and elastic strains, or $\dot{\varepsilon}_{ij} = \dot{\varepsilon}_{ij}^e + \dot{\varepsilon}_{ij}^p$. Since the Helmholtz free energy is defined in Table 3 as $\psi(\varepsilon_{ij}, \varepsilon_{ij}^p, \theta, a^{(k)})$, then its derivative is obtained, similarly as the internal energy. as

$$d\psi(\varepsilon_{ij}, \varepsilon_{ij}^p, \theta, a^{(k)}) = \frac{\partial \psi}{\partial \varepsilon_{ij}^e} d\varepsilon_{ij}^e + \frac{\partial \psi}{\partial \theta} d\theta + \sum_{k=1}^n \frac{\partial \psi}{\partial a^{(k)}} da^{(k)}$$

and properly substituting into Equation 14,

$$\left(\sigma_{ij} - \rho \frac{\partial \psi}{\partial \varepsilon_{ij}^e} \right) \dot{\varepsilon}_{ij}^e - \rho \left(s + \frac{\partial \psi}{\partial \theta} \right) \dot{\theta} + \sigma_{ij} \dot{\varepsilon}_{ij}^p - \sum_{k=1}^n \rho \frac{\partial \psi}{\partial a^{(k)}} \dot{a}^{(k)} - q_i \frac{\theta_{,i}}{\theta} \geq 0 \quad (16)$$

Each of these terms implies a dissipation process, which means that each of these terms must be bigger than zero in order to be thermodynamically admissible. This definition is consistent with the different approaches seen in the literature, since early works done by Coleman and Gurtin, 1967, Germain et al., 1983, and Serrin, 1996; and more recent works done by Houlsby and Puzrin, 2000, Puzrin and Houlsby, 2001, Chaboche, 2003, and Santaoja, 2004. The authors agreed that the first two terms are related to reversible processes, so they cannot generate entropy or dissipation. This means that these two first terms must be zero. When it is done, the equations of state obtained previously are consistent with this appreciation. Also when the generalized thermodynamic forces $A^{(k)}$ are replaced by the negative of the partial derivative the following inequality is obtained:

$$\sigma_{ij} \dot{\varepsilon}_{ij}^p + \sum_{k=1}^n A^{(k)} \dot{a}^{(k)} - q_i \frac{\theta_{,i}}{\theta} \geq 0 \quad (17)$$

All the terms of Equation 17 must be bigger than zero in order to maintain a thermodynamically admissible criterion. This is because the entropy generation in time is always increasing, and then each of its components that produce entropy must be also nonnegative. So, always Equation 18 must be satisfied. If the model is simple, an analytical proof could be done. If this proof is not trivial, a numerical validation of must be done.

$$\sigma_{ij} \dot{\varepsilon}_{ij}^p \geq 0; A^{(k)} \dot{a}^{(k)} \geq 0; -q_i \frac{\theta_{,i}}{\theta} \geq 0 \quad (18)$$

4. NORMALITY RULE AND HOMOGENEITY

Once the entropy generation has been defined as the dissipative rate, several values of this dissipative rate are to be obtained according to the evolution of its internal variables. Since a physical parameter is varying in time, at every step it is moving to a state of minimum energy. Also, a damage surface would be a limit of this energy state. Both considerations must be satisfied at every step in time.

The dissipative rate given by Equation 17 could be separated in two phenomena, one local and other due to heat conduction, as stated in Equation 19. In order to obtain the minimum energy value at every step in time, two concepts will be included in this development. One is the Lagrange multiplier and the other is the yield or failure surface or condition.

$$\gamma = \gamma^{(local)} + \gamma^{(heat)} \geq 0; \text{ where } \gamma^{(local)} = \sigma_{ij} \dot{\varepsilon}_{ij}^p + \sum_{k=1}^n A^{(k)} \dot{a}^{(k)} \geq 0; \gamma^{(heat)} = -q_i \frac{\theta_{,i}}{\theta} \geq 0 \quad (19)$$

4.1 LAGRANGE MULTIPLIER

The Lagrange multiplier is a method for finding the local *extrema* of a function of several variables subject to one or more constraints. This method reduces a problem in n variables with m constraints to a solvable problem in $n+m$ variables without constraints.

For a simple case, observe Figure 5. Here both the dissipation function $\gamma^{(local)}(x, y)$ and a constraint function $h(x, y) = 0$ are defined with two variables x , and y . According to each function value, $0 < d_1 < d_2 < d_3$, several functions in x and y can be built, where the one with minimum energy satisfying its constraint will be the first function that touches the constraint, $\gamma^{(local)} = d_2$. The normal unit vector at this point is the same for both, the function and the constraint.

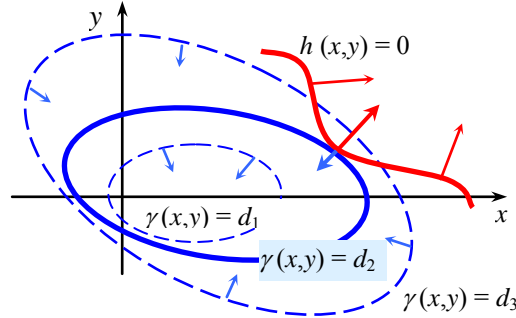


Figure 5: Lagrange multipliers with two variables

An extension of this concept is considered when the extremum of the local dissipative function $\gamma^{(local)}(a^{(k)})$ is constrained by a function $h(a^{(k)})=0$. For this case, the gradient of $\gamma^{(local)}$ must line up with the gradient of h , then $\nabla \gamma^{(local)} + \lambda \nabla h = 0$, so

$$\frac{\partial \gamma^{(local)}}{\partial a^{(k)}} + \lambda \frac{\partial h}{\partial a^{(k)}} = 0, \quad k = 1, 2, \dots, n; h = 0 \quad (20)$$

which leads to $n+1$ equations. Several constraint functions can be considered. For multiple constraints $h^{(1)}, \dots, h^{(m)}$ there would be as many Lagrange multipliers as constraint functions leading to $n+m$ equations, as

$$\frac{\partial \gamma^{(local)}}{\partial a^{(k)}} + \sum_{i=1}^m \lambda^{(i)} \frac{\partial h^{(i)}}{\partial a^{(k)}} = 0; h^{(i)} = 0, \quad \text{for } \begin{cases} k = 1, 2, \dots, n \\ i = 1, 2, \dots, m \end{cases} \quad (21)$$

4.2 YIELD FUNCTION

The following analysis is done for local dissipative functions. The analysis for heat conduction is not included, but could be done in a similar way. From Equation 19, the local dissipative rate is extended as

$$\dot{\gamma}^{(local)}(\varepsilon_{ij}^p, a^{(k)}; \varepsilon_{ij}^p, a^{(k)}) = \sigma_{ij} \varepsilon_{ij}^p + \sum_{k=1}^n A^{(k)} a^{(k)}. \quad \text{The relations } \frac{\partial \dot{\gamma}^{(local)}}{\partial \varepsilon_{ij}^p} = \sigma_{ij}; \frac{\partial \dot{\gamma}^{(local)}}{\partial a^{(k)}} = A^{(k)}, \quad k = 1, 2, \dots, n \quad \text{are}$$

obtained when the partial derivative with respect to its internal variables respectively is performed.

A constraint function is defined with the same internal variables as the dissipative rate function, and thus $h = h(\varepsilon_{ij}^p, a^{(k)}; \varepsilon_{ij}^p, a^{(k)})$ and when the Lagrange multiplier method is used the following relations are obtained

$$\left\{ \frac{\partial \dot{\gamma}^{(local)}}{\partial \varepsilon_{ij}^p} = -\lambda \frac{\partial h}{\partial \varepsilon_{ij}^p} = \sigma_{ij}; \frac{\partial \dot{\gamma}^{(local)}}{\partial a^{(k)}} = -\lambda \frac{\partial h}{\partial a^{(k)}} = A^{(k)}, \quad k = 1, 2, \dots, n; h(\varepsilon_{ij}^p, a^{(k)}; \varepsilon_{ij}^p, a^{(k)}) = 0 \right. \quad (22)$$

A dual constraint function f is now introduced. This dual function is obtained using the Legendre transformation as defined in Equation 4, so

$$f(\hat{\sigma}_{ij}, \hat{A}^{(k)}; \varepsilon_{ij}^p, a^{(k)}) = g(\varepsilon_{ij}^p, a^{(k)}; \varepsilon_{ij}^p, a^{(k)}) - \left[\hat{\sigma}_{ij} \varepsilon_{ij}^p + \sum_{k=1}^n \hat{A}^{(k)} a^{(k)} \right] \quad (23)$$

and the following relations are obtained,

$$\hat{\sigma}_{ij} = \frac{\partial h}{\partial \varepsilon_{ij}^p} = -\frac{1}{\lambda} \sigma_{ij}; \hat{A}^{(k)} = \frac{\partial h}{\partial a^{(k)}} = -\frac{1}{\lambda} A^{(k)}, \quad k = 1, 2, \dots, n \quad (24)$$

When Equations 24 are introduced into Equation 23, the dual function f is redefined as,

$$f(\hat{\sigma}_{ij}, \hat{A}^{(k)}; \varepsilon_{ij}^p, a^{(k)}) = -\hat{\sigma}_{ij} \varepsilon_{ij}^p - \sum_{k=1}^n \hat{A}^{(k)} a^{(k)} \quad (25)$$

or
$$f\left(-\frac{1}{\lambda} \sigma_{ij}, -\frac{1}{\lambda} A^{(k)}; \varepsilon_{ij}^p, a^{(k)}\right) = \sigma_{ij} \left(\frac{1}{\lambda} \varepsilon_{ij}^p\right) + \sum_{k=1}^n A^{(k)} \left(\frac{1}{\lambda} a^{(k)}\right) \quad (26)$$

and employing the definition in Equation 25,

$$f\left(-\frac{1}{\lambda} \sigma_{ij}, -\frac{1}{\lambda} A^{(k)}; \varepsilon_{ij}^p, a^{(k)}\right) = -\frac{1}{\lambda} \left[-\sigma_{ij} \varepsilon_{ij}^p - \sum_{k=1}^n A^{(k)} a^{(k)} \right] = -\frac{1}{\lambda} f(\sigma_{ij}, A^{(k)}; \varepsilon_{ij}^p, a^{(k)}) \quad (27)$$

In mathematics, a homogeneous function is a function with multiplicative scaling behavior. If some of the internal variables of a function ϕ is multiplied by a factor, then the result is multiplied by some power of this factor, or

$$\phi(r x^{(1)}, \dots, r x^{(n)}; \alpha^{(1)}, \dots, \alpha^{(m)}) = r^w \phi(x^{(1)}, \dots, x^{(n)}; \alpha^{(1)}, \dots, \alpha^{(m)}) \quad (28)$$

where Euler's theorem on homogeneous function reads,

$$w \phi(r x^{(1)}, \dots, r x^{(n)}; \alpha^{(1)}, \dots, \alpha^{(m)}) = \sum_{k=1}^n x^{(k)} \frac{\partial \phi(x^{(1)}, \dots, x^{(n)}; \alpha^{(1)}, \dots, \alpha^{(m)})}{\partial x^{(k)}} \quad (29)$$

By inspection it is seen that the definition of a homogeneous function, and the definition of a dual function g are the same for $r = -1/\lambda$ and $w = 1$. So Euler's theorem can be rewritten as

$$f\left(-\frac{1}{\lambda} \sigma_{ij}, -\frac{1}{\lambda} A^{(k)}; \varepsilon_{ij}^p, a^{(k)}\right) = \sigma_{ij} \frac{\partial f(\sigma_{ij}, A^{(k)}; \varepsilon_{ij}^p, \dots, a^{(k)})}{\partial \sigma_{ij}} + \sum_{k=1}^n A^{(k)} \frac{\partial f(\sigma_{ij}, A^{(k)}; \varepsilon_{ij}^p, a^{(k)})}{\partial A^{(k)}} \quad (30)$$

Finally, the following relations are obtained,

$$\varepsilon_{ij}^p = \lambda \frac{\partial f(\sigma_{ij}, A^{(k)}; \varepsilon_{ij}^p, a^{(k)})}{\partial \sigma_{ij}}; a^{(k)} = \lambda \frac{\partial f(\sigma_{ij}, A^{(k)}; \varepsilon_{ij}^p, a^{(k)})}{\partial A^{(k)}}, \quad k = 1, 2, \dots, n \quad (31)$$

When several yield functions are used, an extension of the previous concept is applied. As seen in Equation 20, the number of Lagrange multipliers is the same as the number of yield functions used. Thus, in general the stated relations in Equation can be generalized to

$$\varepsilon_{ij}^p = \sum_{i=1}^m \lambda^{(i)} \frac{\partial f^{(i)}(\sigma_{ij}, A^{(k)}; \varepsilon_{ij}^p, a^{(k)})}{\partial \sigma_{ij}}; a^{(k)} = \sum_{i=1}^m \lambda^{(i)} \frac{\partial f^{(i)}(\sigma_{ij}, A^{(k)}; \varepsilon_{ij}^p, a^{(k)})}{\partial A^{(k)}} \quad (32)$$

where m is the total yield functions, $k = 1, 2, \dots, n$ is the total quantity of thermodynamic forces, and $m \leq n$. Each internal variable rate is related to one yield function, and one function can be related to several internal variables' rates.

5. SUMMARY

In order to define a model the previous definitions are used in sequential steps. These steps could be condensed for the case of small deformations and neglecting temperature effects as:

1. Select the set of state variables: $(\varepsilon_{ij}, \varepsilon_{ij}^p, a^{(k)})$, $k = 1, 2, \dots, n$
2. Define the explicit form for the potentials, i.e., the specific Helmholtz (or Gibbs) free energy and the m -yield function(s): $\psi = \psi(\varepsilon_{ij}, \varepsilon_{ij}^p, a^{(k)})$, $f^{(i)} = f^{(i)}(\sigma_{ij}, A^{(k)}; \varepsilon_{ij}^p, a^{(k)})$, $i = 1, 2, \dots, m$

3. Apply the state equations: $\sigma_{ij} = \rho \frac{\partial \psi}{\partial \varepsilon_{ij}^e}; A^{(k)} = -\rho \frac{\partial \psi}{\partial a^{(k)}}$
4. Apply the normality rule in order to evaluate the internal state variables evolution:

$$\varepsilon_{ij}^p = \sum_{i=1}^m \lambda^{(i)} \frac{\partial f^{(i)}(\sigma_{ij}, A^{(k)})}{\partial \sigma_{ij}}; \dot{a}^{(k)} = \sum_{i=1}^m \lambda^{(i)} \frac{\partial f^{(i)}(\sigma_{ij}, A^{(k)})}{\partial A^{(k)}}$$
5. Verify the homogeneity of each assumed yield function and the satisfaction of the Clausius-Duhem inequality: $\sigma_{ij} \varepsilon_{ij}^p \geq 0; A^{(k)} \dot{a}^{(k)} \geq 0; \lambda^{(i)} > 0$

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