



A thermodynamic framework for constitutive modeling of time- and rate-dependent materials. Part I: Theory

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ABSTRACT

A general thermodynamic-based framework for deriving coupled temperature-dependent viscoelasticity, viscoplasticity, viscodamage, and micro-damage healing constitutive models for constitutive modeling of time- and rate-dependent materials is presented. Principle of virtual power, Clausius–Duhem inequality, and the principle of maximum rate of dissipation are used to construct this general thermodynamic framework. A micro-damage healing natural configuration is introduced to enhance the continuum damage mechanics theories in modeling the healing phenomenon. This healing configuration can be considered as the extension of the well-known Kachanov's effective (undamaged) configuration (Kachanov, 1958). The viscoplasticity loading condition is defined from the microforce balance derived directly from the principle of virtual power. Moreover, for the first time, viscoelasticity, viscodamage, and micro-damage healing microforce balances are derived directly from the principle of virtual power. It is also shown that the generalized non-associative plasticity/viscoplasticity theories can be a direct consequence of postulating the principle of virtual power. The emphasis in this paper is placed on the decomposition of thermodynamic conjugate forces into energetic and dissipative components. It is shown that this decomposition is necessary for accurate estimation of the rate of energy dissipation. The energetic components are related to the Helmholtz free energy, whereas the dissipative components are related to the rate of energy dissipation. This thermodynamic framework is used for deriving more comprehensive viscoelastic, viscoplastic, and viscodamage, and micro-damage healing constitutive models.

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1. Introduction

The mechanical response of a wide range of materials such as polymers, bituminous materials, and soft materials is time- and rate-dependent. Time-dependent materials are defined as those whose mechanical responses depend explicitly on the time (e.g. time of loading). Viscoelastic materials and materials that creep under the constant stresses are good examples of time-dependent materials. The term “rate-dependent” is referred to materials whose behavior implicitly depends on time and explicitly depends on the rate of different measures, such as rate of temperature, loading, and plastic strain. Viscoplastic materials for which the stress depends on the rate of the viscoplastic strain lie within this definition. However, it should be noted that time- and rate-dependency cannot be categorized as inherent material behavior since other factors such as temperature, loading history, and loading rate also affect the time- and rate-dependency. These materials (showing time- and rate-dependent responses under specific circumstances) display all four fundamental responses (i.e. viscoelasticity, viscoplasticity, viscodamage, and micro-damage healing) where contribution of each response strongly depends on the

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temperature and loading conditions. For example, the viscoelastic response could be dominant at low temperatures and stress levels, whereas viscoelastic and viscoplastic responses are dominant at high temperatures. However, the viscodamage (rate-dependent damage) response becomes very important at post peak stress–strain regions, high stress levels, and long loading periods; whereas for some materials, the micro-damage healing could be significant in fatigue loadings. Hence, a robust and comprehensive constitutive model for these materials requires the couplings between temperature, viscoelastic, viscoplastic, viscodamage, and micro-damage healing models to accurately predict their time-, rate-, and temperature-dependent responses. These kinds of constitutive models should also satisfy the laws of thermodynamics.

The development of thermodynamically consistent constitutive models has received great attention in recent decades. Hence, numerous thermodynamic-based models have been proposed in the literature for constitutive modeling of viscoelastic, viscoplastic, and/or viscodamage behavior of different materials such as metals, polymers, soft materials, granular materials, and bio-inspired materials (e.g. Kachanov, 1986; Voyiadjis and Kattan, 1990; Lemaître, 1992; Schapery, 1999; Voyiadjis and Kattan, 1999; Rajagopal and Srinivasa, 2000; Tao et al., 2001; Abu Al-Rub and Voyiadjis, 2003; Boubakar et al., 2003; Cleja-Tigoiu, 2003; Cicekli et al., 2007; Barot et al., 2008; Ghorbel, 2008; Levesque et al., 2008; Voyiadjis et al., 2008; Karra and Rajagopal, 2009; Berbenni et al., 2010; Zhu et al., 2010). Although the literature in developing thermodynamic based constitutive models for materials is rather rich, few attempts are available for coupling all these mechanisms.

Schapery (1969a) derived a single integral equation using the thermodynamics of irreversible processes for constitutive modeling of nonlinear viscoelastic materials. Several authors have extended the one-dimensional (1D) Schapery's constitutive theory to the three-dimensional (3D) viscoelastic models (Henriksen, 1984; Lai and Bakker, 1996; Touati and Cederbaum, 1998; Beijer and Spoomaker, 2002; Haj-Ali and Muliiana, 2004; Levesque et al., 2004). Recently, Levesque et al. (2008) showed that these 3D applications were thermodynamically inconsistent extensions of the 1D Schapery's viscoelastic model, and formulated a thermodynamically consistent 3D Schapery-type viscoelastic model. However, they considered the Cauchy stress tensor as the thermodynamic conjugate force of the total viscoelastic strain tensor. This assumption is valid only for a reversible loading history for which the state variables associated with viscoelastic process remain constant and, hence, is not general.

Several authors have used different approaches and proposed constitutive models to predict the plastic/viscoplastic response of materials (Hashiguchi, 1980; Kaneko and Oyamada, 2000; Hashiguchi, 2005; Hashiguchi and Tsutsumi, 2007; Anandarajah, 2008; Hashiguchi and Ozaki, 2008; La Ragione et al., 2008; Vorobiev, 2008; Voyiadjis et al., 2008; Berbenni et al., 2010; Zhu et al., 2010). To name a few recent works, Hashiguchi (1980) introduced the subloading surface model for the granular materials to describe the rate of the plastic strain due to the rate of the stress inside the yield surface. They used and extended this concept to predict the shear-band inception and thickness (Hashiguchi and Tsutsumi, 2007), tangential plastic strain rate (Hashiguchi, 2005), and plastic softening (Hashiguchi and Ozaki, 2008) in granular materials. Anandarajah (2008) used the concepts of critical state, classical elasto-plasticity, and bounding surface and proposed a multi-mechanism anisotropic model for granular materials. Collard et al. (2010) investigated the role of intra-granular plastic heterogeneities on the strain-hardening response of polycrystals. Kaneko and Oyamada (2000) proposed a viscoplastic model that considers the aging effects in metals. Vorobiev (2008) proposed a thermo-mechanical model to describe the poroelasticity, shear-enhanced compaction, and brittle-ductile transition in dry porous rocks.

Perzyna's viscoplastic model (Perzyna, 1971) is one of the highly used classical models to predict the rate-dependent permanent deformation (i.e. viscoplastic strain) (e.g. Masad et al., 2005; Saadeh et al., 2007; Huang, 2008; Abu Al-Rub et al., 2009). Many researchers have also derived Perzyna's viscoplastic model based on laws of thermodynamics and coupled it to temperature, damage, and/or viscoelasticity to predict more accurately the constitutive behavior of materials (e.g. Dornowski and Perzyna, 2002; Voyiadjis et al., 2003; Abu Al-Rub and Voyiadjis, 2006; Hallberg et al., 2009). These models are usually derived using the overstress concept (Zener and Hollomon, 1944; Malvern, 1951; Perzyna and Korbel, 1998).

However, specific phenomena such as tertiary creep, post-peak behavior of the stress–strain response, fatigue damage, and degradation in the mechanical properties of materials emerge from the changes in the material's microstructure during the deformation. Models based on continuum damage mechanics (CDM) have been effectively used to model degradations in materials due to evolution of cracks and voids (e.g. Kachanov, 1958; Rabotnov, 1969; Lemaître, 1992; Voyiadjis and Kattan, 1992). Several researchers have also coupled viscoelastic and/or plastic/viscoplastic models to isotropic damage to simulate the rate-dependent mechanical response of time-dependent materials (e.g. Hoxha and Homand, 2000; Shao et al., 2003; Masad et al., 2005; Uzan, 2005; Hoxha et al., 2007; Cervenka and Papanikolaou, 2008; Sullivan, 2008; Voyiadjis et al., 2008; Nicot et al., 2009; Zhu et al., 2010; Nicot et al., 2012). However, in most of these works, damage models are not rate-dependent, which poses a challenge in modeling these materials. Several rate-dependent damage models (usually referred to as creep damage) have been proposed in the literature (e.g. Odqvist and Hult, 1961; Cozzarelli and Bernasconi, 1981). However, very few damage models have been coupled to viscoelasticity and viscoplasticity to predict time- and rate-dependent responses of materials. Schapery (1975b,a, 1987) pioneered the formulation of damage models for viscoelastic materials. He also coupled damage to viscoelasticity and to viscoplasticity models (Schapery, 1999). Several researchers have used Schapery's damage model to simulate the mechanical behavior of different materials (e.g. Kim and Little, 1990; Park and Schapery, 1997). However, Schapery's model can only be used to predict viscoplasticity and damage due to tensile stresses and the model also treats the material as a linear viscoelastic material irrespective of temperature and stress levels. Hence, the development of more general viscodamage models and their coupling to temperature, viscoelasticity, and viscoplasticity is necessary for accurate modeling of the rate-dependent mechanical response of time-dependent materials. Recently, Darabi et al. (2011a) proposed a viscodamage model and coupled it to temperature, viscoelasticity, and

viscoplasticity to simulate the mechanical response of bituminous materials. Later, they enhanced their viscodamage model to distinguish between loading in tensile and compressive modes and validated the modified model over another set of experimental data (Darabi et al., 2011b).

Moreover, experimental observations in the last few decades have clearly shown that various classes of engineering materials (e.g. polymers, bitumen, bio-inspired materials, and rocks) have the potential to heal with time and recover part of their strength and stiffness under specific circumstances (e.g. Miao et al., 1995; Kessler and White, 2001; Brown et al., 2002; Reinhardt and Jooss, 2003; Barbero et al., 2005; Guo and Guo, 2006; Bhasin et al., 2008). Although one can find several studies in analyzing different healing processes in a phenomenological point of view (e.g. Jacobsen et al., 1996; Ramm and Biscop, 1998; Ando et al., 2002), few attempts are available for deriving micro-damage healing models based on laws on thermodynamics (e.g. Miao et al., 1995; Barbero et al., 2005). Furthermore, accurate estimation of the rate of energy dissipation is a crucial and challenging task in thermodynamic-based constitutive modeling and should be addressed properly, especially when considering micro-damage healing.

In his celebrated book on continuum thermodynamics, Ziegler (1977) showed that the correct estimation of the rate of energy dissipation requires the decomposition of the thermodynamic conjugate forces into energetic (or quasi-conservative according to his notion) and dissipative components. This general theory is also summarized in his later works (Ziegler, 1983; Ziegler and Wehrli, 1987). In these works, Ziegler showed that the energetic components of the thermodynamic conjugate forces are related to the Helmholtz free energy function, whereas the dissipative components of the thermodynamic conjugate forces are related to the rate of energy dissipation. Therefore, the key assumption in Ziegler's approach states that the constitutive equations for materials can be fully determined by knowledge of the Helmholtz free energy and the dissipation function. Several researchers have used Ziegler's approach to develop constitutive models for different materials. To name a few, Frémond and Nedjar (1996) applied this theory to gradient-dependent damage mechanics. Later, Shizawa and Zbib (1999), and Gurtin and his co-workers (Gurtin, 2003; Gurtin and Anand, 2005, 2009; Gurtin et al., 2007) applied it to gradient-dependent plasticity theories. However, Gurtin and his co-workers did not decompose all thermodynamic conjugate forces into energetic and dissipative components. Moreover, they defined the constitutive expressions for the dissipative conjugate forces as constitutive assumptions instead of deriving those directly from the rate of the energy dissipation. Collins and Houlsby (1997) used the works of Ziegler (1969), Houlsby (1981, 1982), and Modaressi et al. (1994) for modeling the plastic behavior of geomaterials. They showed that when the rate of the plastic energy dissipation is a function of the stress tensor in addition to the plastic strain and its rate, the flow rule is not necessarily associative (Collins and Houlsby, 1997; Collins and Kelly, 2002). However, as it is shown in this paper, there is no need to make these assumptions to obtain the non-associative flow rules for plasticity/viscoplasticity theories. In fact, it is shown here that the non-associative plasticity/viscoplasticity theories are direct consequences of using the principle of virtual power.

This work uses the Clausius–Duhem inequality and the principle of maximum rate of dissipation to derive the desired constitutive model. The Clausius–Duhem inequality is accepted within the entire mechanics community as the thermodynamic requirement which has to be satisfied in all the physical reactions. However, the applicability and validity of the maximum rate of the dissipation for the general cases have been a controversial issue. Onsager (1931a,b) introduced this principle and applied it to the transient heat conduction problem. Afterwards, Ziegler (1961, 1969, 1977) generalized Onsager's formulation and stated that the maximum rate of dissipation holds for arbitrary process obeying the laws of linear nonequilibrium thermodynamics. During the past decades, several researchers have elaborated on the validity and the range of applicability of the maximum rate of dissipation (or more generally maximum entropy production principle) in describing the actual behavior of materials (for more details refer to Kestin and Rice, 1970; Balke, 1976; Lavenda, 1978; Ziegler, 1981; Dewar, 2005; Yang et al., 2005; Martyushev and Seleznev, 2006; Fischer and Svoboda, 2007; Grandy, 2008). In this work, we consider the maximum rate of energy dissipation as a condition to classify the constitutive models. Postulating the maximum rate of energy dissipation condition implies that over all possible different modes of materials' responses (whether dissipative or non-dissipative) with different rates of dissipation, the actual mode is selected as the one with maximum rate of energy dissipation. Therefore, a process could be reversible or non-dissipative only if the selection of dissipative processes is impossible. Although this approach may be criticized on grounds of its applicability to all materials, we believe that it provides a handy tool to solve practical problems and derive robust constitutive models which has been used extensively in the literature for thermodynamic-based constitutive modeling of materials (e.g. Ziegler, 1977; Houlsby, 1982; Svoboda and Turek, 1991; Rajagopal and Srinivasa, 1999; Gill et al., 2001).

Although several researchers have worked and extended the initial work of Ziegler, it is believed that the robustness and capabilities of the Ziegler's thermodynamic approach, specifically, in using the energetic and dissipative conjugate forces to construct a coupled viscoelastic, viscoplastic, viscodamage, and micro-damage healing constitutive model has not been given enough attention. Hence, a general thermodynamic framework is presented in this paper in order to systematically derive various rate-dependent constitutive models with emphasis on the decomposition of thermodynamic conjugate forces into energetic and dissipative components. Also, a systematic procedure for determining the energetic and dissipative components directly from the Helmholtz free energy function and the rate of energy dissipation, respectively, is presented. It is also shown in this paper that the viscoelastic, viscoplastic, viscodamage, and micro-damage healing microforce balances that are derived based on the principle of virtual power yield general partial differential equations that govern the viscoelastic, viscodamage, and micro-damage healing processes. The capabilities and robustness of the presented thermodynamic framework is shown through several examples which derive Schapery-type thermo-viscoelastic model, Perzyna-type

thermo-viscoplastic model, the thermo-viscodamage model proposed by Darabi et al. (2011a), and the micro-damage healing model proposed by Abu Al-Rub et al. (2010).

Note that in all subsequent sections indices m and n range from 1 to N_{int}^{ve} (the maximum number of internal state variables associated with the viscoelastic processes) while the other indices range from 1 to 3. Moreover, bold letters indicate that variables are tensors or matrices.

2. Natural Configurations and Transformation Hypotheses

2.1. Isotropic damage

In this section, we recall the definition of the damage variable in one-dimension as originally proposed by Kachanov (1958), and further developed by other researchers (Odqvist and Hult, 1961; Rabotnov, 1969; Lemaître and Chaboche, 1990). Consider a uniform bar subjected to a uniaxial tensile load T as shown in Fig. 1(a). The total cross-sectional area of the bar in this configuration (i.e. nominal or damaged configuration) is A and it is assumed that both cracks and voids appear as damage and form a total damage area of A^D . Kachanov (1958) and Rabotnov (1969) introduced the fictitious undamaged (effective) configuration by removing all types of damage, including both cracks and voids, from the bar as shown in Fig. 1(b). The effective cross-sectional area in the undamaged configuration is denoted by \tilde{A} that is in fact the total cross-sectional area without the damaged areas ($\tilde{A} = A - A^D$). The bars in both damaged and undamaged configurations are subjected to the same tensile force T , such that:

$$\sigma A = \tilde{\sigma} \tilde{A} \quad (1)$$

where σ is the stress in the damaged configuration and $\tilde{\sigma}$ is the stress in the effective configuration. The relationship between σ and the $\tilde{\sigma}$ can now be obtained using Eq. (1) and the relations between the cross-sectional areas, such that:

$$\sigma = (1 - \phi) \tilde{\sigma} \quad (2)$$

where ϕ is the so-called damage variable or the damage density (i.e. the area of micro-cracks and micro-voids per unit area) which starts from $\phi = 0$ (even for initial damaged material) ending with $\phi = 1$ (for complete rupture). Similarly, a relation between the effective stress tensor $\tilde{\sigma}$ and the stress tensor in the damaged configuration σ for the case of isotropic damage (i.e. scalar damage variable) can be written as follows:

$$\sigma_{ij} = (1 - \phi) \tilde{\sigma}_{ij} \quad (3)$$

2.2. Healing natural configuration

Here we recall the definition of the healing natural configuration as introduced by Abu Al-Rub et al. (2010) and Darabi et al. (2012). The classical assumption in Eqs. (2) and (3) is that the damage density is irreversible. Hence, an increasing function with time is usually postulated to describe the damage variable ϕ (Kachanov, 1958, 1986; Lemaître, 1992; Kattan and Voyiadjis, 1993; Krajcinovic, 1996). However, as discussed in the introduction section, some engineering materials have the potential to heal and recover part of their strength and stiffness under specific conditions such as resting periods during fatigue loading and under hydrostatic pressure. Hence, a proper CDM framework should be able to describe, besides the damage, the changes in the materials microstructure during the micro-damage healing process. To achieve this goal, we extend the classical effective configuration by introducing a natural configuration named the *healing configuration* as shown in Fig. 2.

Fig. 2(a) shows a bar subjected to a uniaxial tensile load T at the current time t . During the loading–unloading processes, some new micro-cracks and micro-voids nucleate and propagate upon satisfaction of the damage nucleation and growth conditions. On the other hand, for certain materials (e.g. polymers, bituminous materials, and biological materials) some

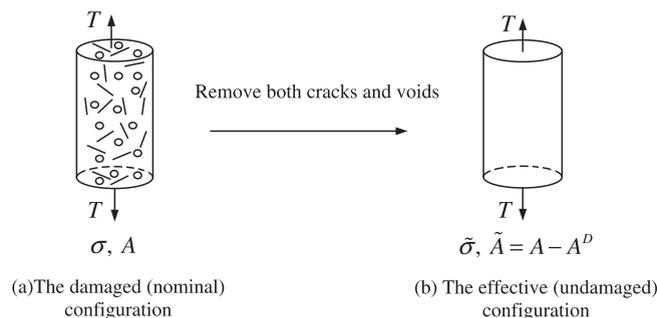


Fig. 1. Definition of the classical effective configuration in continuum damage mechanics (Abu Al-Rub and Voyiadjis, 2003).

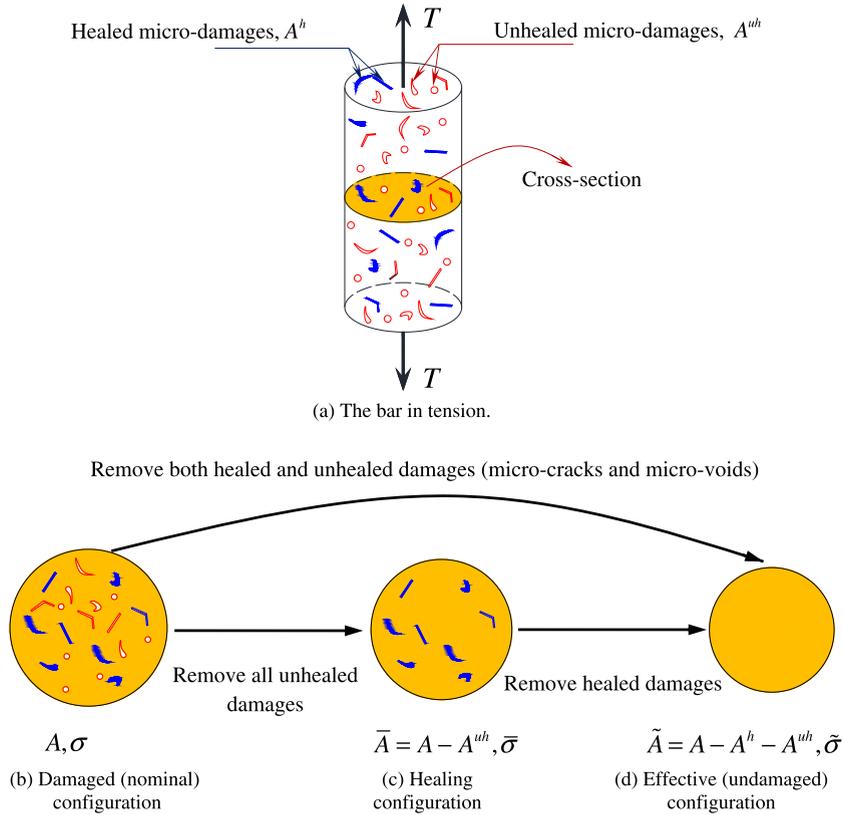


Fig. 2. Extension of the effective stress concept in continuum damage mechanics to continuum damaged-healing mechanics (Darabi et al., 2012).

of these micro-cracks may heal during the resting period (or the unloading process). Therefore, we divide the total cross-sectional area of the bar A of the cylinder into three parts: (a) the area that has not been damaged (i.e. intact area), \tilde{A} , which can be considered as the effective (undamaged) area in CDM; (b) the area of unhealed micro-cracks and voids, A^{uh} ; and (c) the area of the micro-cracks and micro-voids that have been healed during the unloading process or the rest period, A^h . Thus, we can define three configurations: (1) the damaged configuration with the total cross-sectional area of A (Fig. 2(b)); (2) the healing configuration resulting from removing unhealed micro-voids and micro-cracks from the total cross-sectional area and has the total area of \bar{A} (Fig. 2(c)); and (3) the effective configuration that results from removing also the healed micro-cracks from the healing configuration and has the total area of \tilde{A} (Fig. 2(d)). The relationships between the cross-sectional areas in these three configurations can be written as follows:

$$A = \tilde{A} + A^D = \bar{A} + A^{uh} \tag{4}$$

where A^D is the total damaged area including all unhealed and healed damages, such that:

$$A^D = A^h + A^{uh} \tag{5}$$

As it is argued in classical CDM, cracks and voids cannot carry load. Hence, the load is carried by the area of the intact materials (i.e. \tilde{A}) and the area of those healed micro-cracks (i.e. A^h). In other words, both damaged (nominal) and healing configurations carry the same tensile load T , such that:

$$T = \sigma A = \bar{\sigma} \bar{A} \tag{6}$$

where the superimposed “-” in this paper designates the healing configuration. Now, we define the damage density variable ϕ as the ratio of the total damaged area over the total cross-sectional area and the healing variable h as the ratio of the area of the healed micro-cracks over the total damaged area, such that:

$$\phi = \frac{A^D}{A}; \quad h = \frac{A^h}{A^D} \tag{7}$$

For the cases when micro-damage healing is not considered, ϕ is the classical irreversible damage density variable ranging from $0 \leq \phi \leq 1$, which is interpreted as the micro-damage density such that $\phi = 0$ indicates no damage and $\phi = 1$ indicates complete damage (or failure). However, when micro-damage healing is included, ϕ is interpreted as an internal

state variable representing the damage history such that A^D is the cumulative damaged area. On the other hand, h is the healing internal variable defined as the ratio of the cumulative area of healed micro-damages over the cumulative damaged area. Therefore, h represents the healed fraction of the total damaged area. The healing variable ranges from $0 \leq h \leq 1$; $h = 0$ for no healing and $h = 1$ when all micro-cracks and micro-voids are healed. We can now define the relationship between the stresses in the damaged and healing configurations by substituting Eqs. (4), (5), (7)₁, and (7)₂ into Eq. (6), such that:

$$\sigma = [1 - \phi(1 - h)]\bar{\sigma} \quad (8)$$

Eq. (8) extends the classical definition in Eq. (2) to include micro-damage healing. Similarly, the relation between the healing stress tensor $\bar{\sigma}$ and the stress tensor in the damaged configuration σ for the case of isotropic damage and isotropic healing can be written as follows:

$$\sigma_{ij} = [1 - \phi(1 - h)]\bar{\sigma}_{ij} \quad (9)$$

Comparing Eqs. (2) and (9) allows us to define the effective damage density $\bar{\phi}$ which considers the effects of damage nucleation, growth, and micro-damage healing, such that:

$$\bar{\phi} = \phi(1 - h) \quad (10)$$

Note that when $h = 0$ (i.e. $\bar{\phi} = \phi$), Eqs. (2) and (9) are identical which implies that no healing has occurred in the material. On the other hand, when $h = 1$ (i.e. $\bar{\phi} = 0$), the stress tensor in the damaged configuration σ , the effective stress tensor $\bar{\sigma}$, and the healing stress tensor $\bar{\sigma}$ are the same, which implies that all micro-cracks have been healed; and hence, the material has completely recovered its strength and stiffness.

Several studies are available in the literature where a single damage variable is used to account for micro-damage healing as well as the damage effects (e.g. Alfredsson and Stigh, 2004). In these cases, the damage evolution is considered to be dependent on time and loading history to account for healing. While this is an elegant approach to consider the micro-damage healing effect, we believe that considering another physically-based internal state variable (i.e. h) provides a more general approach for modeling the micro-damage healing process in the materials. The previous thermodynamic-based micro-damage healing models, whether using a single or several state variables to represent damage and healing, are developed for a specific micro-damage healing mechanism and are not general. They are either developed to model the autonomous micro-damage healing mechanism (e.g. Barbero et al., 2005) or they are applicable to the materials that heal during the rest period and unloading (e.g. Miao et al., 1995; Alfredsson and Stigh, 2004). However, the current approach is more general and treats the micro-damage healing generally as the reduction of the damage density regardless of the specific type of healing. It should be noted that the micro-damage healing evolution function will be different depending on the healing mechanism and on the material type.

Moreover, assuming a single damage variable to capture both damage and healing effects assigns a single thermodynamic driving force (i.e. conjugate to the introduced internal variable) to be responsible for both damage and healing evolutions. However, we clearly present physically-based variables (i.e. ϕ and h) to capture damage and micro-damage healing effects. This would be very beneficial for the cases where the driving forces for the damage and healing mechanisms are not similar. Another motivation to consider a separate state variable to account for healing process is the flexibility of this approach to carefully consider the stored and dissipates energies during damage and healing mechanisms. Unlike the previous approaches (e.g. Miao et al., 1995; Alfredsson and Stigh, 2004; Barbero et al., 2005; Voyiadjis et al., 2011), the current approach allows the clear distinction between energetic and dissipative components of the damage and micro-damage healing thermodynamic conjugate forces in order to guarantees a positive-definite rate of energy dissipation.

It is noteworthy that the healing variable in Eq. (10) has a similar effect to the stiffness-recovery parameter introduced in the work of Lee and Fenves (1998) for modeling the stiffness recovery in concrete materials during the transition from tension to compression loading. However, the physics behind the stiffness-recovery parameter by Lee and Fenves (1998) is different than the current proposed micro-damage healing variable h . Lee and Fenves (1998) interpreted the area of healed micro-cracks in Eq. (7)₂, A^h , as the area of closed micro-cracks (not healed) during the loading transition from tension to compression. Therefore, the current proposed micro-damage healing variable is more general as it can be interpreted as a crack-closure parameter or as a micro-damage healing parameter, but with a different evolution law, depending on the intended application (refer to Darabi et al., 2012 for more details).

Moreover, the following relationship between the stress tensors in the healing and effective configurations is obtained if one assumes that the tensile forces in the effective and healing configurations are the same (i.e. $\bar{\sigma}\bar{A} = \bar{\sigma}\bar{A}$ in Fig. 2), such that:

$$\bar{\sigma}_{ij} = \left[\frac{1 - \phi(1 - h)}{1 - \phi} \right] \sigma_{ij} \quad (11)$$

Eq. (11) clearly shows that the stress tensors in the healing and effective configurations will be the same only for two cases: (1) the damage variable is zero (i.e. $\phi = 0$), where in this case the stress tensors in the effective and healing configurations (i.e. $\bar{\sigma}$ and $\bar{\sigma}$) will be the same as the stress tensor in the damaged configuration (i.e. σ) since damage has not started yet; (2) micro-damage healing variable is zero (i.e. $h = 0$), where in this case the stress tensors in the effective and healing configurations will be the same since micro-damage healing is not considered. For other cases, the stress tensor in the fictitious effective configuration will be always greater than the stress tensor in the healing configuration (i.e. $\bar{\sigma} \geq \bar{\sigma}$). In other words,

the effective configuration (Fig. 2(d)) is obtained by removing the healed micro-damage areas from the healing configuration (Fig. 2(c)) such that these healed micro-damages can tolerate load and carry stress in the healing configuration. Therefore, the stress tensor in the effective configurations should be magnified comparing to the stress tensor in the healing configuration in order to compensate for the stresses carried by the removed healed micro-damages.

2.3. Transformation hypotheses and additive decomposition of strain tensor

A common argument in CDM based on the effective stress space is that once a material is damaged further loading only affects the undamaged (intact) material skeleton (c.f. Voyiadjis et al., 2004). We can make a similar argument when the micro-damage healing process is in effect. Hence, we argue that once a material is damaged further loading only affects the intact and healed portions of the material. In other words, further loading is carried out by the material in the healing configuration shown in Fig. 2. We use this motivation for development of our constitutive model in the healing configuration (i.e. in terms of $\bar{\sigma}$).

In this work, small deformations and a separable material (i.e. the viscoelastic compliance is independent of viscoplasticity internal state variables) are assumed. Thus, the total deformation can be additively decomposed into viscoelastic (recoverable) and viscoplastic (irrecoverable) components, such that:

$$\boldsymbol{\varepsilon}_{ij} = \boldsymbol{\varepsilon}_{ij}^{ve} + \boldsymbol{\varepsilon}_{ij}^{vp} \quad (12)$$

where $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}^{ve}$, and $\boldsymbol{\varepsilon}^{vp}$ are the total, viscoelastic, and viscoplastic strain tensors, respectively. For small deformations, the total strain $\boldsymbol{\varepsilon}$ is defined in terms of the displacement vector \mathbf{u} as

$$\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad (13)$$

We assume the same additive strain decomposition in the healing configuration, such that:

$$\bar{\boldsymbol{\varepsilon}}_{ij} = \bar{\boldsymbol{\varepsilon}}_{ij}^{ve} + \bar{\boldsymbol{\varepsilon}}_{ij}^{vp} \quad (14)$$

It is worth noting that the additive decomposition of the total strain tensor into the elastic/viscoelastic and plastic/viscoplastic components and considering those identical respectively to the experimentally measured recoverable and irrecoverable strains has been a debating issue over the past years especially for geomaterials and frictional materials (e.g. Darve et al., 1995; Collins and Houslyby, 1997; Collins, 2005; Nicot and Darve, 2006). Collins (2005) introduced the concept of 'frozen' elastic energy for geomaterials and stated that the decomposition of the applied work into recoverable elastic energy and irrecoverable plastic energy is not valid at the continuum scale. He showed that some of the micro-level elastic energy does not recover during a stress cycle because of the highly heterogeneous nature of stress and deformation fields in geomaterials. Nicot and Darve (2006) stated that the elastic behavior of geomaterials depends on the fabric of medium which evolves with the evolution of the plastic strain and made similar conclusions. However, for small deformation theories and specific types of the materials (e.g. bituminous materials and polymer composites), the changes in the microstructure due to small plastic strain can be negligible since the particles (inclusions) are embedded in the matrix and are not in direct contact. Nicot and Darve (2006) conducted a micro-structural analysis by representing a hypothetical geomaterial as particles in contact with each other. They showed that part of the elastic energy will not recover during an elementary stress cycle. The main assumption in their work is that the contacts between the particles are the main mechanism of load transfer and deformation. However, for bituminous materials and polymer composites, the matrix plays a crucial role in load transfer and deformation mechanism, such that few particles might be in direct contact for small deformations. The experimental observations also confirm this mechanism since the tensile and compressive strengths of these materials are not very different (e.g. the tensile strength of bituminous materials is about 80% of their compressive strength). Although establishing a macroscopic definition of elastic/viscoelastic strains yields more accurate predictions in geomaterials, the establishment of such definition and relating elastic/viscoelastic and plastic/viscoplastic strains to the experimentally measured recoverable and irrecoverable strains are challenging tasks that may lead to more complex constitutive equations (e.g. Chang and Hicher, 2005; Nicot and Darve, 2006). Extending the current formulation to the large deformation theories with micro-structural considerations will be the subject of a future work by the authors.

By using the proposed healing stress concept, a transformation hypothesis is required to relate the stress and strain tensors ($\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$) in the damaged configuration to the stress and strain tensors in the healing configuration ($\bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{\varepsilon}}$). Several transformation hypotheses have been proposed in the literature to relate strains and stiffness moduli in the effective and damaged configurations. One of the first transformation hypotheses is the strain equivalence hypothesis (Lemaître and Chaboche, 1990). Based on this hypothesis, the total strain in the damaged and effective configurations are the same (i.e. $\boldsymbol{\varepsilon}_{ij} = \bar{\boldsymbol{\varepsilon}}_{ij}$). This hypothesis makes the numerical implementation of constitutive models very simple. However, it results in a linear relationship between the stiffness moduli in the damaged and effective configuration. Sidoroff (1981) proposed another transformation hypothesis based on equivalency of the elastic energy in the effective and damaged configurations that results in a quadratic relationship between the stiffness moduli in the effective and damaged configurations. This hypothesis has been used extensively in the literature (see e.g. Voyiadjis and Kattan, 1993; Zhu and Cescotto, 1995; Lemaître et al., 2000; Voyiadjis et al., 2003). Another transformation hypothesis that can be used for the constitutive models accompanied with

dissipative processes such as plasticity is based on the equivalency of the power in the effective and damaged configurations. Lee et al. (1985) proposed this hypothesis and assumed that the expended power associated with the plasticity process is equivalent in the damaged and effective configurations. Voyiadjis and Thiagarajan (1997) also used this hypothesis and proposed an uncoupled plastic-anisotropic damage model. Later, Voyiadjis et al. (2004) adopted this hypothesis for viscoplasticity and derived a gradient-dependent viscoplasticity and anisotropic-viscodamage constitutive model.

In this work, we adopt the power transformation hypothesis, which states that the power expenditure associated with each type of dissipative process in the damaged configuration is equal to the corresponding power expenditure in the effective configuration. However, we extend this hypothesis for correlating the power in the damaged and healing configurations. Postulating this hypothesis along with using continuum damage-healing mechanics based on the healing stress space are both numerically and physically interesting. In other words, using the healing stress space eliminates numerical complexities associated with the direct couplings of the damage and micro-damage healing models to the rest of the constitutive model; whereas, power-correlating hypothesis makes these simplifications physically sound since it allows the accurate estimation of the dissipated power in the healing stress space (healing natural configuration).

By postulating this hypothesis, we assume that the expended power resulting from the viscoelastic and viscoplastic processes are the same in the damaged and healing configurations. In this study, we assume isotropic damage and isotropic micro-damage healing variables in order to present the general steps of the proposed thermodynamic framework in a much clearer and simpler way. Anisotropic damage and anisotropic micro-damage healing will be considered in a future work. Applying the power equivalence hypothesis for the isotropic damage and isotropic micro-damage healing cases yields the following relations between different components of the strain tensor in the damaged and healing configurations, such that:

$$\dot{\hat{\epsilon}}_{ij}^{vp} = [1 - \phi(1 - h)]\dot{\epsilon}_{ij}^{vp}; \quad \dot{\hat{\epsilon}}_{ij}^{ve} = [1 - \phi(1 - h)]\dot{\epsilon}_{ij}^{ve} \quad (15)$$

where the superimposed dot in Eq. (15) and all equations in this paper designates the derivation with respect to time. Substituting Eq. (15) into Eq. (12) yields the relationship between the total strain tensor in the damaged and healing configurations, such that:

$$\dot{\hat{\epsilon}}_{ij} = [1 - \phi(1 - h)]\dot{\epsilon}_{ij} \quad (16)$$

The strain rates $\dot{\epsilon}$, $\dot{\epsilon}^{ve}$, and $\dot{\epsilon}^{vp}$ in Eqs. (15) and (16) represent the rates of the total strain, viscoelastic strain, and viscoplastic strain tensors in the damaged configuration, respectively; whereas the strain rates $\dot{\hat{\epsilon}}$, $\dot{\hat{\epsilon}}^{ve}$, and $\dot{\hat{\epsilon}}^{vp}$ represent their corresponding counterparts in the healing configuration, respectively.

We will use Eqs. (14)–(16) in the following sections to express the constitutive models in the healing configuration.

3. Thermodynamic framework

3.1. Internal and external expenditures of power

Axioms of equilibrium and thermodynamics should be satisfied to formulate a proper material constitutive model. In this section, expressions for the internal and external expenditures of power are defined following the framework of Gurtin (2003), but with the consideration of viscoelasticity, damage, and micro-damage healing. Definition of the internal and external expenditures of power is often thought to be very fixed. However, Frémond and Nedjar (1996) modified the definition of the classical form of the internal virtual power by including, in addition to the classical terms involving strain rates, the damage rate and its gradient. They also modified the expression of the external expenditure of power by including the effects of the external sources of the body and surface damage forces to explain the microscopic movements that produce damage. Based on these modifications, they formulated an elastic-gradient-dependent damage model. We use a similar line of thought here to derive constitutive equations that couple viscoelastic (creep and relaxation properties), viscoplastic (rate-dependent plasticity), viscodamage (rate-dependent damage), and micro-damage healing models to explain the time- and rate-dependent mechanical response of materials.

Experimental observations show that specific materials such as bituminous materials undergo healing process during the rest period (i.e. the external loading is removed from the body). During the rest period the external loading is removed and therefore the external power could become zero. However, the micro-damage healing process partially continues by consuming some of the energies stored inside the body. The complete healing occurs once some external energy in the form of heat is supplied to the body. This temperature loading speeds up the healing process and in some cases is essential for the complete healing process. In these cases, the temperature change and evolution will be extremely important and cannot be ignored (e.g. Cardona et al., 1999). This can be verified by studying the effect of temperature on the healing process (e.g. Reinhardt and Jooss, 2003; Kessler, 2007; Little and Bhasin, 2007).

The present treatment is limited to local viscoelasticity, viscoplasticity, damage, and micro-damage healing where higher-order nonlocal gradient-dependent variables will be introduced in a future work. Let Γ be an arbitrary sub-body and let \mathbf{n} denotes the outward unit normal to the boundary $\partial\Gamma$ of Γ . In this work, we consider the displacement vector \mathbf{u} , the viscoelastic strain tensor $\boldsymbol{\epsilon}^{ve}$, the viscoplastic strain tensor $\boldsymbol{\epsilon}^{vp}$, the effective plastic strain p , the damage density ϕ , the healing variable h , and the absolute temperature T , such that the generalized virtual motions will be the set of $\{\mathbf{u}, \boldsymbol{\epsilon}^{ve}, \boldsymbol{\epsilon}^{vp}, \dot{p}, \dot{\phi}, \dot{h}, \dot{T}\}$. It is assumed that these virtual motions are, momentarily, independent. However, the dependency

among these virtual motions will be established later. It should be noted that the rate of temperature \dot{T} has been added to the conventional velocity variables to ensure the generality of the thermodynamic framework and to capture the endothermic nature of the healing process. The internal expenditure of power is assumed to be characterized by the Cauchy stress tensor $\boldsymbol{\sigma}$ defined over Γ for all times, the backstress \mathbf{X} associated with kinematic hardening and conjugate to $\boldsymbol{\varepsilon}^{vp}$, the viscoplastic hardening stress R associated with isotropic hardening and conjugate to p , the damage force Y conjugate to ϕ , the micro-damage healing force H conjugate to h , N_{int}^{ve} – thermodynamic forces χ_n conjugated to the N_{int}^{ve} – of phenomenological internal state variables associated with viscoelastic process, ξ_n ($n = 1, \dots, N_{int}^{vi}$, $N_{int}^{vi} \geq 1$), and the generalized thermodynamic force a^{int} conjugate to \dot{T} . Thus, the expenditure of the internal power can be written as:

$$P_{int} = \int_{\Gamma} \left(\boldsymbol{\sigma}_{ij} \dot{\varepsilon}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \chi_n \dot{\xi}_n + X_{ij} \dot{\varepsilon}_{ij}^{vp} + R \dot{p} + Y \dot{\phi} + H \dot{h} + a^{int} \dot{T} \right) dV \quad (17)$$

In Eq. (17), \dot{p} is the rate of the equivalent viscoplastic strain, which is defined by:

$$\dot{p} = \sqrt{2 \dot{\varepsilon}_{ij}^{vp} \dot{\varepsilon}_{ij}^{vp} / 3} \quad (18)$$

The additional generalized thermodynamic force a^{int} is defined similar to Cardona et al. (1999). Eq. (17) is based on the concept that the power expended by each kinematical field be expressible in terms of an associated force system consistent with its own balance. The first two terms in Eq. (17) represent the internal power generated because of the viscoelastic processes. The third and the fourth terms represent the internal power generated by the viscoplastic process. The third term accounts for internal power expenditure by the backstress \mathbf{X} (the residual stress) which introduces anisotropic viscoplastic hardening effects, whereas the fourth term is the internal power due to viscoplastic isotropic hardening. The fifth and the sixth terms are the internal power expended by the damage and micro-damage healing processes, respectively. Finally, the last term defines the internal power expended due to the temperature change. However, the kinematical fields in Eq. (17) are no longer independent and, therefore, special care is taken in the following in order to properly account for their couplings. Moreover, although the two state variables ε_{ij}^{vp} and p are dependent, they introduce different physics such that the viscoplastic strain ε_{ij}^{vp} results in kinematic hardening in the viscoplasticity model whereas the effective plastic strain p results in isotropic hardening in the viscoplastic model (c.f. Abu Al-Rub et al., 2007; Voyiadjis and Abu Al-Rub, 2007).

It is noteworthy that the internal state variables associated with the viscoelastic process (ξ_n) are considered as hidden state variables. These hidden state variables are associated with internal phenomena such as chain mobility in polymers and cause the evolution of the viscoelastic strain ε_{ij}^{ve} which is an observable variable that can be measured by experiments. However, although these hidden state variables result in the evolution of the viscoelastic strain tensor, their contribution to the stored and dissipated energies should be considered for more accurate estimation of these energies in viscoelastic materials (as will be shown in the next sections). Schapery (1966) defines these viscoelastic internal state variables as the generalized coordinates which could be physically interpreted as the variables representing molecular configurations in polymers or location of interstitial atoms in metals (please refer to Schapery (1964, 1966) for more details).

On the other hand, the external expenditure of power is defined in terms of the macroscopic body force \mathbf{b} , a macroscopic surface traction \mathbf{t} , and the inertial forces. Therefore, the external expenditure of the power can be written as follows:

$$P_{ext} = \int_{\Gamma} \mathbf{b}_i \dot{u}_i dV + \int_{\partial\Gamma} \mathbf{t}_i \dot{u}_i dA - \int_{\Gamma} \rho \ddot{u}_i \dot{u}_i dV \quad (19)$$

where ρ is the material density.

3.2. Principle of virtual power

The principle of the virtual power is the assertion that, given any sub-body Γ , the virtual power expended on Γ by materials or bodies exterior to Γ (i.e. external power) is equal to the virtual power expended within Γ (i.e. internal power). Eqs. (17) and (19) represent the actual expenditures of the power during a kinematical process. The virtual expenditure of the power can be defined when the prescribed fields are replaced by virtual ones. Hence, we can write internal and external expenditures of virtual power as:

$$\hat{P}_{int} = \int_{\Gamma} \left(\boldsymbol{\sigma}_{ij} \delta \dot{\varepsilon}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \chi_n \delta \dot{\xi}_n + X_{ij} \delta \dot{\varepsilon}_{ij}^{vp} + R \delta \dot{p} + Y \delta \dot{\phi} + H \delta \dot{h} + a^{int} \delta \dot{T} \right) dV \quad (20)$$

$$\hat{P}_{ext} = \int_{\Gamma} \mathbf{b}_i \delta \dot{u}_i dV + \int_{\partial\Gamma} \mathbf{t}_i \delta \dot{u}_i dA - \int_{\Gamma} \rho \delta \ddot{u}_i \delta \dot{u}_i dV \quad (21)$$

where \hat{P}_{int} and \hat{P}_{ext} represent internal and external expenditures of virtual power, respectively. Note that the kinematical fields $\delta \dot{\mathbf{u}}$, $\delta \dot{\boldsymbol{\varepsilon}}^{ve}$, $\delta \dot{\boldsymbol{\varepsilon}}^{vp}$, $\delta \dot{p}$, $\delta \dot{\phi}$, $\delta \dot{h}$, and $\delta \dot{\xi}$, and $\delta \dot{T}$ in Eqs. (20) and (21) are virtual, where δ is the variation operator.

According to the principle of the virtual power, the external virtual power (Eq. (20)) should be balanced by the internal expenditure of virtual power (Eq. (21)), such that:

$$\hat{P}_{int} = \hat{P}_{ext} \quad (22)$$

Let \mathbf{N} be a second-order tensor representing the unit direction of the viscoplastic strain tensor, $\dot{\boldsymbol{\varepsilon}}^{vp}$, such that:

$$N_{ij} = \frac{\dot{\varepsilon}_{ij}^{vp}}{\|\dot{\varepsilon}_{ij}^{vp}\|} = \sqrt{\frac{2}{3}} \frac{\dot{\varepsilon}_{ij}^{vp}}{\dot{p}} \quad (23)$$

where Eq. (18) is used in obtaining the right-hand-side of Eq. (23).

After substituting the time rate of Eqs. (12) and (13), along with Eqs. (20) and (21) into Eq. (22), using the divergence theorem, making use of Eq. (23), and some mathematical manipulations, the following equation is obtained:

$$\int_{\Gamma} \left[(\sigma_{ijj} + b_i - \rho \ddot{u}_i) \delta \dot{u}_i + \left(\sqrt{\frac{3}{2}} (\sigma_{ij} - X_{ij}) N_{ij} - R \right) \delta \dot{p} - Y \delta \dot{\phi} - \sum_{n=1}^{N_{int}^{pe}} \chi_n \delta \dot{\xi}_n \right] dV - \int_{\Gamma} (H \delta \dot{h} + a^{int} \delta \dot{T}) dV + \int_{\partial \Gamma} (t_i - \sigma_{ij} n_j) \delta \dot{u}_i dA = 0 \quad (24)$$

The fields Γ , $\delta \mathbf{u}$, $\delta \dot{p}$, $\delta \dot{\phi}$, and $\delta \dot{\xi}$ may be arbitrary specified if and only if

$$\sigma_{ijj} + b_i = \rho \ddot{u}_i, \quad \text{in } \Gamma \quad (25)$$

$$t_i = \sigma_{ij} n_j, \quad \text{on } \partial \Gamma \quad (26)$$

$$\sqrt{\frac{3}{2}} (\sigma_{ij} - X_{ij}) N_{ij} - R = 0, \quad \text{in } \Gamma \quad (27)$$

$$Y = 0, \quad \text{in } \Gamma \quad (28)$$

$$\chi_n = 0, \quad \text{in } \Gamma, n \in [1, \dots, N_{int}^{vi}] \quad (29)$$

Eq. (25) expresses the local stress equilibrium equation or the macroforce balance, Eq. (26) defines the macroscopic boundary traction as the density of the surface forces introduced, Eq. (27) is the viscoplastic microforce balance according to notion of Gurtin (2003) that will be used for deriving the viscoplasticity yield surface in the subsequent sections, and Eq. (28) defines the damage microforce balance (Frémond and Nedjar, 1996) that will be used in deriving the viscodamage nucleation and growth conditions. We also define Eq. (29) as the viscoelastic microforce balance, which is new and non-classical for viscoelastic materials. As we will show in this paper, this simple balance law results in the general partial differential equation that explains the viscoelastic processes in materials.

Substituting Eqs. (25)–(29) into Eq. (24) yields:

$$\int_{\Gamma} (H \delta \dot{h} + a^{int} \delta \dot{T}) dV = 0 \quad (30)$$

From which it is immediately implied that:

$$H \delta \dot{h} + a^{int} \delta \dot{T} = 0, \quad \text{in } \Gamma \quad (31)$$

Eq. (31) is defined as the *micro-damage healing microforce balance*. This new and non-classical balance law will be used to define the micro-damage healing evolution function and condition. This equation shows the dependency of the internal power of healing on the temperature rate. The simplest assumption is to set $\delta \dot{T}$ and $\delta \dot{h}$ to be independent variables, such that we can write:

$$H = 0; \quad a^{int} = 0 \quad (32)$$

This assumption, as we will see later, is valid for the ideal case of completely self-healing materials. In this case, both damage and healing processes will be considered reversible and no energy is dissipated during the damage/healing processes. However, the more general approach is to accept the dependency of the healing rate on the rate of temperature around the healing process zone, such that Eq. (31) is valid in its coupled form. This is due to the fact that the complete healing process is accompanied by the energy absorption and can be considered analogous to endothermic processes (i.e. the process in which the system absorbs energy from the surroundings in the form of heat). In other words, Eq. (31) shows that in the absence of the external power, the healing process absorbs the required energy for the healing process from its surroundings in the form of heat and therefore changes the temperature around the healing process zone, at least during the healing process. This is in agreement with the endothermic nature of the healing process. Eq. (31) can be explained even for the isothermal conditions for which the body Γ is in contact with a reservoir maintaining a constant temperature. In this case, the healing process continues by absorbing heat energy from its surrounding and causes the temperature drop within the healing process zone. The reservoir will then compensate for this temperature drop by supplying the heat to the body Γ guaranteeing the isothermal condition. However, the time scale for achieving the isothermal condition is on the order of the healing process time which makes it impossible, for practical purposes, to neglect this transient region during the healing process. In other words, even for the isothermal condition, there will be a time scale in the order of the required time for the healing process to occur for which the isothermal condition is not maintained anymore. Moreover, the rate of this heat

absorption is directly correlated to the rate of the healing process. Therefore, as the first approximation, we assume here a linear relationship between the rate of the temperature change and the healing rate (i.e. $a^{int}\delta\dot{T} = -K\delta\dot{h}$), such that the micro-damage healing microforce balance can be simplified as follows for any arbitrary $\delta\dot{T}$ or $\delta\dot{h}$:

$$H - K = 0 \tag{33}$$

where K can be defined as the rate of the heat energy that the healing process absorbs from the surroundings in order to reach the unit rate for the healing variable (or equivalently, rate of the heat energy per rate of the healing variable). In this work, we will use Eq. (33) to derive the micro-damage healing condition and the evolution equation for h .

3.3. Principle of virtual power in the healing configuration

We wish to derive the constitutive model in the fictitious healing configuration since the common argument in CDM is that once the material is damaged, further loading can only affect the undamaged and, in this case, the healed portion of the material skeleton. Obviously, before the material is damaged, the effective healing and damaged configurations are identical.

As it was mentioned in the previous section, the healing configuration is defined as a fictitious state where the unhealed and partially-healed damages in the material are removed. Hence, damage does not contribute to the internal expenditure of power in the healing configuration, whereas further healing may occur to the partially-healed micro-cracks. Therefore, in the healing configuration, $\bar{\sigma}$, \bar{X} , \bar{R} , H , a^{int} , and N_{int}^{ve} – thermodynamic forces $\bar{\chi}_n$ conjugated to the N_{int}^{ve} – of phenomenological internal state variables associated with viscoelastic process, $\bar{\xi}_n$ ($n = 1, \dots, N_{int}^{vi}$; $N_{int}^{vi} \geq 1$) contribute to the internal expenditure of power, such that:

$$\widehat{P}_{int} = \int_{\Gamma} \left(\bar{\sigma}_{ij} \delta \dot{\epsilon}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \bar{\chi}_n \delta \dot{\xi}_n + \bar{X}_{ij} \delta \dot{\epsilon}_{ij}^{vp} + \bar{R} \delta \dot{p} + H \dot{h} + a^{int} \dot{T} \right) dV \tag{34}$$

where \widehat{P}_{int} is the internal expenditure of virtual power in the healing configuration, and $\dot{p} = \sqrt{2 \dot{\epsilon}_{ij}^{vp} \dot{\epsilon}_{ij}^{vp}} / 3 = [1 - \phi(1 - h)] \dot{p}$ by substituting Eq. (15) into Eq. (18). However, as it was shown, the damage and micro-damage healing conditions in the damaged configuration are always null (i.e. $Y = 0$ and $H - K = 0$; Eqs. (28) and (33), respectively). Hence, by adopting the power equivalence transformation hypothesis (presented in Section 2.3) and also using Eqs. (28) and (33), or its general form presented in Eq. (31), it can be easily shown that Eqs. (20) and (34) are the same, such that:

$$\widehat{P}_{int} = \widehat{P}_{int} \tag{35}$$

This can be verified by substituting Eqs. (9), (15), (16), (28), and (31) into Eq. (34) to obtain Eq. (20). It is noteworthy that the power equivalence hypothesis is used for all components of the viscoelastic power in the damaged and healing configurations (i.e. $\sum_{n=1}^{N_{int}^{ve}} \bar{\chi}_n \dot{\xi}_n = \sum_{n=1}^{N_{int}^{ve}} \chi_n \dot{\xi}_n$ and $\bar{\sigma}_{ij} \dot{\epsilon}_{ij}^{ve} = \sigma_{ij} \dot{\epsilon}_{ij}^{ve}$).

Substituting Eqs. (9), (33), (34), and (35) into Eq. (22), along with using the time rate of the strain decomposition in the healing configuration, and performing some mathematical manipulations yield the following equations:

$$[1 - \phi(1 - h)] \bar{\sigma}_{ij,j} + b_i = \rho \ddot{u}_i, \quad \text{in } \Gamma \tag{36}$$

$$t_i = [1 - \phi(1 - h)] \bar{\sigma}_{ij} n_j, \quad \text{on } \partial\Gamma \tag{37}$$

$$\sqrt{\frac{3}{2}} (\bar{\sigma}_{ij} - \bar{X}_{ij}) \bar{N}_{ij} - \bar{R} = 0, \quad \text{in } \Gamma \tag{38}$$

$$\bar{\chi}_n = 0, \quad \text{in } \Gamma, \quad n \in [1, \dots, N_{int}^{vi}] \tag{39}$$

Substituting Eq. (9) into Eqs. (36) and (37) shows that these two equations are the same as Eqs. (25) and (26), respectively. Eq. (39) defines the balance law for internal work of viscoelastic process in the healing configuration. Moreover, Eq. (38) shows the microforce balance in the healing configuration, where:

$$\bar{N}_{ij} = \frac{\dot{\epsilon}_{ij}^{vp}}{\|\dot{\epsilon}_{ij}^{vp}\|} = \sqrt{\frac{2}{3}} \frac{\dot{\epsilon}_{ij}^{vp}}{\dot{p}} \tag{40}$$

Substituting Eq. (16) into Eq. (40) yields:

$$\bar{N}_{ij} = N_{ij} \tag{41}$$

We will use Eq. (38) for deriving the viscoplasticity yield surface in the healing configuration.

It should be noted that one of the challenges in deriving thermodynamic-based plasticity/viscoplasticity theories is that it is commonly believed that the thermodynamic laws, as presented in this section, lead to associative plasticity/viscoplasticity which are not applicable to pressure sensitive materials. However, one of the objectives of this work is to derive the generalized non-associative viscoplasticity theories solely based on the presented thermodynamic laws and without assuming extra

assumptions (e.g. assuming a viscoplastic potential function that is different from the yield surface to ensure the non-associative theories). In Appendix I, we will show that the generalized non-associative plastic/viscoplastic theories are direct consequences of principle of virtual power and there is no need to postulate extra assumptions to achieve non-associative theories. The formulations presented in Appendix A will then be used in the subsequent sections to derive generalized non-associative viscoplastic theories.

3.4. Internal state variables and Clausius–Duhem inequality

In developing the thermodynamic-based constitutive equations, it is assumed that the state of materials is characterized by suitable internal state variables that implicitly describe important microstructural mechanisms that affect the macroscopic behavior of the material under specific loading and (initial) boundary conditions. The Helmholtz free energy is considered as the thermodynamic state potential depending on the internal state variables. Here, we assume the Helmholtz free energy Ψ to depend on the viscoelastic strain $\bar{\epsilon}^{ve}$, the viscoplastic strain $\bar{\epsilon}^{vp}$, the equivalent viscoplastic strain \bar{p} in the healing configuration, the damage density ϕ , the micro-damage healing variable h , N_{int}^{vi} of internal state variables related to the viscoelastic processes $\bar{\xi}_n$ ($n = 1, \dots, N_{int}^{vi}$; $N_{int}^{vi} \geq 1$), and absolute temperature T . This assumption is consistent with the assumed expression for the internal power, Eq. (17). Hence, the Helmholtz free energy density function Ψ can be expressed as:

$$\Psi = \Psi(\bar{\epsilon}_{ij}^{ve}, \bar{\xi}_n, \bar{\epsilon}_{ij}^{vp}, \bar{p}, \phi, h, T) \quad (42)$$

Again, we mention that the internal state variables associated with the viscoelastic processes, $\bar{\xi}_n$, are considered as hidden variables. These hidden variables are associated with internal phenomenon such as the chain mobility in polymers and cause the evolution of the viscoelastic strain $\bar{\epsilon}_{ij}^{ve}$ which is an observable variable that can be measured experimentally.

By combining the first and second laws of thermodynamics (i.e. balance of energy and entropy imbalance, respectively) and also applying the conservation of mass, (i.e. $\dot{\rho} + \rho \dot{u}_{i,i} = 0$), the Clausius–Duhem inequality for non-isothermal conditions can be written as follows (c.f. Lemaître and Chaboche, 1990):

$$\int_{\Gamma} [\rho(\dot{\Psi} + \eta\dot{T}) + \frac{1}{T} q_i T_{,i}] dV \leq P_{ext} = P_{int} \quad (43)$$

where η is the specific entropy. Eq. (43) is valid for all sub-regions Γ . Substituting Eq. (34) into Eq. (43) by replacing the virtual fields with the real ones, noting that the sub-region Γ is arbitrary, and substituting Eq. (33) yield the following local form of the Clausius–Duhem inequality:

$$\bar{\sigma}_{ij} \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \bar{\chi}_n \dot{\bar{\xi}}_n + \bar{X}_{ij} \dot{\bar{\epsilon}}_{ij}^{vp} + \bar{R} \dot{\bar{p}} + (H - K) \dot{h} - \rho(\dot{\Psi} + \eta\dot{T}) - \frac{1}{T} q_i T_{,i} \geq 0 \quad (44)$$

which defines the rate of the energy dissipation per unit volume, Π . However, the damage balance law (i.e. $Y = 0$) is null according to Eq. (28). Hence, we can easily include this term into Eq. (44) without changing the values of the rate of energy dissipation per unit volume. As we will see in the next sections, adding this null term will substantially simplify the derivation of the damage condition. Hence, we can rewrite Eq. (44) as:

$$\bar{\sigma}_{ij} \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \bar{\chi}_n \dot{\bar{\xi}}_n + \bar{X}_{ij} \dot{\bar{\epsilon}}_{ij}^{vp} + \bar{R} \dot{\bar{p}} + Y \dot{\phi} + (H - K) \dot{h} - \rho(\dot{\Psi} + \eta\dot{T}) - \frac{1}{T} q_i T_{,i} \geq 0 \quad (45)$$

Taking the time derivative of the Helmholtz free energy, Eq. (42), gives:

$$\dot{\Psi} = \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{ve}} \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \left(\frac{\partial \Psi}{\partial \bar{\xi}_n} \dot{\bar{\xi}}_n \right) + \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{vp}} \dot{\bar{\epsilon}}_{ij}^{vp} + \frac{\partial \Psi}{\partial \bar{p}} \dot{\bar{p}} + \frac{\partial \Psi}{\partial \phi} \dot{\phi} + \frac{\partial \Psi}{\partial h} \dot{h} + \frac{\partial \Psi}{\partial T} \dot{T} \quad (46)$$

Substituting Eq. (46) into the local Clausius–Duhem inequality (Eq. (45)) yields:

$$\left(\bar{\sigma}_{ij} - \rho \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{ve}} \right) \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \left(\bar{\chi}_n - \rho \frac{\partial \Psi}{\partial \bar{\xi}_n} \right) \dot{\bar{\xi}}_n + \left(\bar{X}_{ij} - \rho \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{vp}} \right) \dot{\bar{\epsilon}}_{ij}^{vp} + \left(\bar{R} - \rho \frac{\partial \Psi}{\partial \bar{p}} \right) \dot{\bar{p}} + \left(Y - \rho \frac{\partial \Psi}{\partial \phi} \right) \dot{\phi} + \left(H - K - \rho \frac{\partial \Psi}{\partial h} \right) \dot{h} - \rho \left(\eta + \frac{\partial \Psi}{\partial T} \right) \dot{T} - \frac{1}{T} q_i T_{,i} \geq 0 \quad (47)$$

From Eq. (47) the following classical thermodynamic state law for entropy is defined:

$$\eta = - \frac{\partial \Psi}{\partial T} \quad (48)$$

such that the rate of the energy dissipation Π from Eqs. (47) and (48) can be written as:

$$\Pi = \left(\bar{\sigma}_{ij} - \rho \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{ve}} \right) \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \left(\bar{\chi}_n - \rho \frac{\partial \Psi}{\partial \bar{\xi}_n} \right) \dot{\bar{\xi}}_n + \left(\bar{X}_{ij} - \rho \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{vp}} \right) \dot{\bar{\epsilon}}_{ij}^{vp} + \left(\bar{R} - \rho \frac{\partial \Psi}{\partial \bar{p}} \right) \dot{\bar{p}} + \left(Y - \rho \frac{\partial \Psi}{\partial \phi} \right) \dot{\phi} + \left(H - K - \rho \frac{\partial \Psi}{\partial h} \right) \dot{h} - \frac{1}{T} q_i T_{,i} \geq 0 \quad (49)$$

Eq. (49) contains terms that are only a function of the Helmholtz free energy which can be defined as the energetic (or quasi-conservative) components of the thermodynamic conjugate forces (Ziegler, 1983; Gurtin, 2003), such that:

$$\bar{\sigma}_{ij}^{\text{ene}} \equiv \rho \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{ve}}; \quad \bar{\chi}_n^{\text{ene}} \equiv \rho \frac{\partial \Psi}{\partial \bar{\xi}_n}, \quad n \in [1, \dots, N_{\text{int}}^{ve}] \quad (50)$$

$$\bar{X}_{ij}^{\text{ene}} \equiv \rho \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{vp}}; \quad \bar{R}^{\text{ene}} \equiv \rho \frac{\partial \Psi}{\partial \bar{p}} \quad (51)$$

$$Y^{\text{ene}} \equiv \rho \frac{\partial \Psi}{\partial \phi} \quad (52)$$

$$H^{\text{ene}} \equiv \rho \frac{\partial \Psi}{\partial h} \quad (53)$$

where $\bar{\sigma}_{ij}^{\text{ene}}$, $\bar{\chi}_n^{\text{ene}}$, $\bar{X}_{ij}^{\text{ene}}$, \bar{R}^{ene} , Y^{ene} , and H^{ene} are energetic components of the thermodynamic forces conjugate to $\bar{\epsilon}^{ve}$, $\bar{\xi}_n$, $\bar{\epsilon}^{vp}$, \bar{p} , ϕ , and h , respectively. Substituting Eqs. (50)–(53) into the equation for the rate of energy dissipation gives Eq. (49):

$$\Pi = \left(\bar{\sigma}_{ij} - \bar{\sigma}_{ij}^{\text{ene}} \right) \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{\text{int}}^{ve}} \left(\bar{\chi}_n - \bar{\chi}_n^{\text{ene}} \right) \dot{\bar{\xi}}_n + \left(\bar{X}_{ij} - \bar{X}_{ij}^{\text{ene}} \right) \dot{\bar{\epsilon}}_{ij}^{vp} + \left(\bar{R} - \bar{R}^{\text{ene}} \right) \dot{\bar{p}} + \left(Y - Y^{\text{ene}} \right) \dot{\phi} + \left(H - K - H^{\text{ene}} \right) \dot{h} - \frac{1}{T} q_i T_{,i} \geq 0 \quad (54)$$

Eq. (54) shows that the rate of energy dissipation resulting from different mechanisms (i.e. viscoelasticity, viscoplasticity, viscodamage, and micro-damage healing) is positive only if the thermodynamic conjugate forces have dissipative components as well. Hence, we can rewrite Eq. (54) as follows:

$$\Pi = \bar{\sigma}_{ij}^{\text{dis}} \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{\text{int}}^{ve}} \bar{\chi}_n^{\text{dis}} \dot{\bar{\xi}}_n + \bar{X}_{ij}^{\text{dis}} \dot{\bar{\epsilon}}_{ij}^{vp} + \bar{R}^{\text{dis}} \dot{\bar{p}} + Y^{\text{dis}} \dot{\phi} + \left(H^{\text{dis}} - K \right) \dot{h} - \frac{1}{T} q_i T_{,i} \geq 0 \quad (55)$$

where $\bar{\sigma}_{ij}^{\text{dis}}$, $\bar{\chi}_n^{\text{dis}}$, $\bar{X}_{ij}^{\text{dis}}$, \bar{R}^{dis} , Y^{dis} , and H^{dis} are dissipative components of the thermodynamic forces conjugate to the rate of effective viscoelastic strain tensor, $\dot{\bar{\epsilon}}^{ve}$, the rate of the viscoelasticity state variables, $\dot{\bar{\xi}}_n$, the rate of viscoplastic strain tensor, $\dot{\bar{\epsilon}}^{vp}$, the rate of the equivalent viscoplastic strain in the effective configuration, $\dot{\bar{p}}$, the rate of the damage density, $\dot{\phi}$, and the rate of the micro-damage healing variable, \dot{h} , respectively, and defined as follows:

$$\bar{\sigma}_{ij}^{\text{dis}} = \bar{\sigma}_{ij} - \bar{\sigma}_{ij}^{\text{ene}}; \quad \bar{\chi}_n^{\text{dis}} = \bar{\chi}_n - \bar{\chi}_n^{\text{ene}}; \quad n \in [1 \dots N_{\text{int}}^{ve}] \quad (56)$$

$$\bar{X}_{ij}^{\text{dis}} = \bar{X}_{ij} - \bar{X}_{ij}^{\text{ene}}; \quad \bar{R}^{\text{dis}} = \bar{R} - \bar{R}^{\text{ene}} \quad (57)$$

$$Y^{\text{dis}} = Y - Y^{\text{ene}} \quad (58)$$

$$H^{\text{dis}} = H - H^{\text{ene}} \quad (59)$$

Therefore, in the current paper, energetic means that the thermodynamic conjugate forces are derived from the Helmholtz free energy function whereas dissipative means that they are derived from the rate of energy dissipation function. Therefore, in order to formulate constitutive equations for the energetic and dissipative conjugate forces, we need to know: (1) how the material stores energy which helps in assuming a mathematical form for the Helmholtz free energy, and (2) how the material dissipates energy which helps in assuming a mathematical form for the rate of energy dissipation. Furthermore, the rate of energy dissipation (Eq. (49)) naturally enforces the decomposition of the stress tensor into energetic and dissipative components. As we will see later in this paper, this decomposition results in a more comprehensive relation between the stress and the viscoelastic strain compared to the classical relations for linearly/nonlinearly viscoelastic materials.

It is noteworthy to mention that the Clausius–Duhem inequality also enforces the decomposition of the specific entropy η into energetic specific entropy (i.e. $\eta^{\text{ene}} = -\frac{\partial \Psi}{\partial T}$) and the dissipative specific entropy (i.e. $\eta^{\text{dis}} = \eta - \eta^{\text{ene}}$) which is related directly to the rate of energy dissipation. However, we do not use this decomposition for the specific entropy in this paper and we assume the classical thermodynamic law for entropy as in Eq. (48) with $\dot{\eta}^{\text{dis}} = 0$.

Let us assume for a moment that neither damage/healing nor viscoplasticity occur in the material (i.e. $\dot{\bar{p}} = 0$, $\dot{\phi} = 0$, and $\dot{h} = 0$) in order to explain the common argument that has been made in the literature for substituting the total stress instead of its energetic component in Eq. (50) [c.f. Levesque et al. (2008)]. Therefore, assuming *isothermal* conditions as well, the Clausius–Duhem inequality in Eq. (47) reduces to the following form:

$$\left(\bar{\sigma}_{ij} - \rho \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{ve}} \right) \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{\text{int}}^{ve}} \left(\bar{\chi}_n - \rho \frac{\partial \Psi}{\partial \bar{\xi}_n} \right) \dot{\bar{\xi}}_n \geq 0 \quad (60)$$

The commonly used argument states that the Clausius–Duhem inequality (Eq. (60)) is valid for all load histories. So, let the loading history to be a hypothetical reversible loading history such that the viscoelastic internal state variables remain constant (i.e. $\dot{\bar{\xi}}_n = 0$). Under this load history the second term of the inequality in Eq. (60) vanishes and the following constitutive law is obtained:

$$\bar{\sigma}_{ij} = \rho \frac{\partial \Psi}{\partial \bar{\epsilon}_{ij}^{ve}} \quad (61)$$

However, we believe that this argument is not consistent. The reason is that the material is viscoelastic, and hence, the state variables $\bar{\xi}_n$ are not independent of the viscoelastic strains $\bar{\epsilon}^{ve}$ and they evolve even under the unloading process. In other words, both $\bar{\epsilon}^{ve}$ and $\bar{\xi}_n$ evolve during the viscoelastic process whether it is loading or unloading. Hence, a more consistent framework is to admit the decomposition of the stress tensor into energetic and dissipative components as in Eq. (56) such that Eq. (61) defines the thermodynamic law for the energetic component.

Apart from the energy dissipation due to viscoelastic and viscoplastic processes, it is also interesting to look at the energy dissipation due to damage and micro-damage healing processes more closely. In this work, we assume that a specific location within the material at a specific time t can either undergo the damage process or undergo the micro-damage healing process. Therefore, the rate of the micro-damage healing variable is zero during the damage process and vice versa. The rates of the energy dissipation during the damage process Π^{tvd} and during the micro-damage healing process Π^{th} are expressed as follows:

$$\Pi^{tvd} = (Y - Y^{ene})\dot{\phi} \geq 0; \quad \Pi^{th} = (H - H^{ene})\dot{h} - K\dot{h} \geq 0 \quad (62)$$

During the damage process the rate of the micro-damage healing variable is zero and therefore the micro-damage healing process does not contribute to the rate of energy dissipation in this case. Eq. (62)₁ shows that the value of the expended internal power due to the damage process (i.e. $Y\dot{\phi}$) should be greater than the rate of the stored energy inside the material due to the damage hardening (i.e. $Y^{ene}\dot{\phi}$). Therefore, part of the expended internal power due to damage is dissipated (i.e. Π^{tvd}). On the other hand, Eq. (62)₂ represents the rate of energy dissipation during the micro-damage healing process. A closer look at Eq. (62)₂ shows that part of the required internal power for the micro-damage healing process is provided by the stored energy due to the micro-damage healing process (i.e. $H^{ene}\dot{h}$). This released energy (provided by the decrease in the stored energy, $H^{ene}\dot{h}$) is derived from the surface free energy on the faces of the cracks that participate in the healing process as well as from, in certain systems, the increase in configurational entropy. For example, in a bitumen system, the introduction of a crack face probably establishes a preferred orientation of aliphatic, polynuclear aromatic, and naphthenic aromatics. During the healing process a reorganization of these phases or components across the crack interface contributes to some degree to the re-establishment of strength, healing, resulting in an increase in configurational entropy and a decrease in free energy. In fact, Bhasin et al. (2011) established, using molecular dynamics, that the composition of the bitumen affects the rate of reorganization across an interface. This released energy is spent for partial micro-damage healing process. The extra required energy for the micro-damage healing process (i.e. $K\dot{h}$) comes from the heat energy absorbed from the areas surrounding the healing process zone (i.e. $a^{int}\dot{T}$). For the hypothetical completely self-healing materials this extra energy is not required (i.e. $K=0$), such that the damage and micro-damage healing processes does not dissipate energy and can be considered as reversible processes. However, this condition does not occur in reality.

Next section focuses on deriving the thermodynamic laws for the dissipative components of the thermodynamic conjugate forces.

3.5. Maximum rate of the energy dissipation principle

As it was shown in the previous section, the estimation of the rate of energy dissipation requires the decomposition of the thermodynamic conjugate forces into energetic and dissipative components (Ziegler, 1977, 1983; Ziegler and Wehrli, 1987; Frémond and Nedjar, 1996; Shizawa and Zbib, 1999; Gurtin, 2003; Anand et al., 2005; Gurtin and Anand, 2005; Abu Al-Rub et al., 2007; Gurtin and Anand, 2009; Lele and Anand, 2009; Voyiadjis and Deliktas, 2009). However, in all of these works, except for the works of Ziegler (1977, 1983) and Shizawa and Zbib (1999), the constitutive equations for the dissipative components are merely constitutive assumptions and are not derived based on the laws of thermodynamics. However, in this work, the dissipative components of thermodynamic conjugate forces are determined directly from the rate of energy dissipation by using the maximum rate of energy dissipation principle. Eq. (55) shows that the rate of the energy dissipation can be decomposed into its thermo-viscoelastic, Π^{tve} , thermo-viscoplastic, Π^{tvp} , thermo-viscodamage, Π^{tvd} , thermo-healing, Π^{th} , and thermal, Π^{th} , components, such that:

$$\Pi = \Pi^{tve} + \Pi^{tvp} + \Pi^{tvd} + \Pi^{th} + \Pi^{th} \geq 0 \quad (63)$$

where Π^{tve} , Π^{tvp} , Π^{tvd} , Π^{th} , and Π^{th} are given by:

$$\Pi^{tve} = \bar{\sigma}_{ij}^{dis} \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{int}^{ve}} \bar{\lambda}_n^{dis} \dot{\bar{\xi}}_n \geq 0 \quad (64)$$

$$\Pi^{tvp} = \bar{X}_{ij}^{dis} \dot{\bar{\epsilon}}_{ij}^{vp} + \bar{R}^{dis} \dot{\bar{p}} \geq 0 \quad (65)$$

$$\Pi^{tvd} = Y^{dis} \dot{\phi} \geq 0 \quad (66)$$

$$\Pi^{th} = (H^{dis} - K)\dot{h} \geq 0 \quad (67)$$

$$\Pi^{th} = -\frac{1}{T} q_i T_{,i} \geq 0 \quad (68)$$

Obviously, Eqs. (64)–(68) are more strict constraints for obtaining a positive-definite dissipation than that in Eq. (55). Now, constraint conditions are needed in order to maximize the rate of energy dissipation. This can be achieved by defining the following constraint conditions:

$$D^{ve} = \Pi^{tve} - \left(\bar{\sigma}_{ij}^{\text{dis}} \dot{\bar{\epsilon}}_{ij}^{ve} + \sum_{n=1}^{N_{\text{int}}^{ve}} \bar{\chi}_n^{\text{dis}} \dot{\bar{\zeta}}_n \right) = 0 \quad (69)$$

$$D^{vp} = \Pi^{tvp} - \left(\bar{X}_{ij}^{\text{dis}} \dot{\bar{\epsilon}}_{ij}^{vp} + \bar{R}^{\text{dis}} \dot{\bar{p}} \right) = 0 \quad (70)$$

$$D^{vd} = \Pi^{tvd} - Y^{\text{dis}} \dot{\phi} = 0 \quad (71)$$

$$D^H = \Pi^{tH} - (H^{\text{dis}} - K) \dot{h} = 0 \quad (72)$$

$$D^{\text{th}} = \Pi^{\text{th}} + \frac{1}{T} q_i T_{,i} = 0 \quad (73)$$

Hence, the following objective functions Ω^{ve} , Ω^{vp} , Ω^{vd} , Ω^H , and Ω^{th} with their corresponding Lagrange multipliers Λ^{ve} , Λ^{vp} , Λ^{vd} , Λ^H , and Λ^{th} subjected to the constraint $D^{ve} = 0$, $D^{vp} = 0$, $D^{vd} = 0$, $D^H = 0$, and $D^{\text{th}} = 0$, respectively, are defined, such that:

$$\Omega^{ve} = \Pi^{tve} - \Lambda^{ve} D^{ve} \quad (74)$$

$$\Omega^{vp} = \Pi^{tvp} - \Lambda^{vp} D^{vp} \quad (75)$$

$$\Omega^{vd} = \Pi^{tvd} - \Lambda^{vd} D^{vd} \quad (76)$$

$$\Omega^H = \Pi^{tH} - \Lambda^H D^H \quad (77)$$

$$\Omega^{\text{th}} = \Pi^{\text{th}} - \Lambda^{\text{th}} D^{\text{th}} \quad (78)$$

Maximizing the above objective functions by using the necessary conditions implies:

$$\frac{\partial \Omega^{ve}}{\partial \dot{\bar{\epsilon}}_{ij}^{ve}} = 0; \quad \frac{\partial \Omega^{ve}}{\partial \dot{\bar{\zeta}}_n} = 0; \quad \frac{\partial \Omega^{vp}}{\partial \dot{\bar{\epsilon}}_{ij}^{vp}} = 0; \quad \frac{\partial \Omega^{vp}}{\partial \dot{\bar{p}}} = 0; \quad \frac{\partial \Omega^{vd}}{\partial \dot{\phi}} = 0; \quad \frac{\partial \Omega^H}{\partial \dot{h}} = 0; \quad \frac{\partial \Omega^{\text{th}}}{\partial (q_i/T)} = 0 \quad (79)$$

Substituting Eqs. (74)–(78) into Eq. (79) yields the following conjugate laws for the dissipative forces, such that:

$$\bar{\sigma}_{ij}^{\text{dis}} = \hat{\Lambda}^{ve} \frac{\partial \Pi^{tve}}{\partial \dot{\bar{\epsilon}}_{ij}^{ve}}; \quad \bar{\chi}_n^{\text{dis}} = \hat{\Lambda}^{ve} \frac{\partial \Pi^{tve}}{\partial \dot{\bar{\zeta}}_n}, \quad n \in [1, \dots, N_{\text{int}}^{ve}] \quad (80)$$

$$\bar{X}_{ij}^{\text{dis}} = \hat{\Lambda}^{vp} \frac{\partial \Pi^{tvp}}{\partial \dot{\bar{\epsilon}}_{ij}^{vp}}; \quad \bar{R}^{\text{dis}} = \hat{\Lambda}^{vp} \frac{\partial \Pi^{tvp}}{\partial \dot{\bar{p}}} \quad (81)$$

$$Y^{\text{dis}} = \hat{\Lambda}^{vd} \frac{\partial \Pi^{tvd}}{\partial \dot{\phi}} \quad (82)$$

$$H^{\text{dis}} - K = \hat{\Lambda}^H \frac{\partial \Pi^{tH}}{\partial \dot{h}} \quad (83)$$

$$T_{,i} = -\hat{\Lambda}^{\text{th}} \frac{\partial \Pi^{\text{th}}}{\partial (q_i/T)} \quad (84)$$

where

$$\hat{\Lambda}^{ve} = 1 - \frac{1}{\Lambda^{ve}}, \quad \hat{\Lambda}^{vp} = 1 - \frac{1}{\Lambda^{vp}}, \quad \hat{\Lambda}^{vd} = 1 - \frac{1}{\Lambda^{vd}}, \quad \hat{\Lambda}^H = 1 - \frac{1}{\Lambda^H}, \quad \hat{\Lambda}^{\text{th}} = 1 - \frac{1}{\Lambda^{\text{th}}} \quad (85)$$

The Lagrange multipliers in Eq. (85) can be determined by substituting Eqs. (80)–(84) respectively into Eqs. (64)–(68).

It is noteworthy that other constraints such as the viscoplastic microforce balance (Eq. (27) or (38)), the viscodamage microforce balance (Eq. (28)), the micro-damage healing microforce balance (Eq. (33)), and the viscoelastic microforce balance (Eq. (29)) can also be applied to the objective functions which requires determination of several Lagrange multipliers. Although applying more constraints to the objective function results in a more comprehensive solution for dissipative components of the thermodynamic conjugate forces, it makes the problem more complex.

This section concludes the general thermodynamic framework for determining the energetic and dissipative components of the thermodynamic conjugate forces. In the following sections, we focus on showing the capabilities of the presented thermodynamic framework through an example that derives a temperature-dependent viscoelastic, viscoplastic, viscodamage, and micro-damage healing constitutive model.

4. Viscoelastic–viscoplastic–viscodamage–healing constitutive laws

Formulating a general thermodynamic framework that properly estimates the stored and dissipative energies during the viscoelasticity, viscoplasticity, damage, and healing processes is one of the most challenging tasks. This issue has been

addressed in this work by decomposing the thermodynamic conjugate forces into energetic and dissipative components and enforcing the positive-definite rate of dissipation for these processes. However, careful experimental studies should be performed to come out with the proper forms of the Helmholtz free energy and rate of energy dissipation functions based on the material type. An experimental protocol that can be used systematically in order to select proper forms of Helmholtz free energy and rate of energy dissipation functions is highly desirable.

In this section, we use the thermodynamic framework presented in the previous sections to derive thermo-viscoelastic, thermo-viscoplastic, thermo-viscodamage, and thermo-healing constitutive equations. The objective is to derive thermodynamic consistent Schapery-type viscoelastic model, Perzyna-type viscoplastic model, damage model proposed by Darabi et al. (2011a), and a micro-damage healing model proposed by Abu Al-Rub et al. (2010). Subsequently, a systematic procedure for identifying the model parameters associated with the derived constitutive model will be presented in the second part of this paper (Darabi et al., submitted for publication). The calibrated model will then be validated against an extensive experimental data including creep, creep-recovery, triaxial, constant strain rate tests (strain rates ranging from $10^{-2}/s$ to $10^{-5}/s$), and repeated creep-recovery tests at different temperatures, stress levels, loading times, and unloading (or resting) times.

Assuming a decoupled or a separable material, we decompose the Helmholtz free energy into thermo-viscoelastic, thermo-viscoplastic, thermo-viscodamage, and healing components, such that:

$$\Psi(\bar{\epsilon}_{ij}^{ve}, \bar{\epsilon}_{ij}^{vp}, \bar{p}, \phi, h, \zeta_n, T) = \Psi^{tve}(\bar{\epsilon}_{ij}^{ve}, \zeta_n, T) + \Psi^{tvp}(\bar{\epsilon}_{ij}^{vp}, \bar{p}, T) + \Psi^{tvd}(\phi, T) + \Psi^{th}(h, T) \quad (86)$$

where Ψ^{tve} , Ψ^{tvp} , Ψ^{tvd} , and Ψ^{th} are thermo-viscoelastic, thermo-viscoplastic, thermo-viscodamage, and thermo-healing components of the Helmholtz free energy.

4.1. Thermo-viscoelasticity constitutive equations

Schapery (1969b) used the thermodynamics of irreversible processes and developed a single integral constitutive model for nonlinear viscoelastic materials. Schapery made his viscoelastic model nonlinear by introducing the stress and/or strain-dependent scalars at various steps during the development of the constitutive theory. Recently, Levesque et al. (2008) extended the Schapery's nonlinear viscoelastic model for 3D applications based on laws of thermodynamics. Here, we follow the procedure of Levesque et al. (2008) to derive the viscoelasticity model and couple it to viscoplasticity, viscodamage, and micro-damage healing models. However, we express the formulation in the healing configuration and we also decompose the thermodynamic conjugate forces into energetic and dissipative components which results in a more general relationship between the stress and the viscoelastic strain, as argued in previous sections. Moreover, we make use of the viscoelastic microforce balance (Eq. (39)) to derive viscoelastic constitutive equations.

Here, we consider both the viscoelastic strain tensor and the viscoelastic internal state variables $\bar{\zeta}_n$ to contribute to the viscoelastic component of the Helmholtz free energy. Hence, the thermo-viscoelastic component of the Helmholtz free energy can be assumed as follows:

$$\rho \Psi^{tve} = \left[\frac{1}{2} a_0(\bar{\epsilon}^{ve}) L_{ijkl}^{(1)} \bar{\epsilon}_{ij}^{ve} \bar{\epsilon}_{kl}^{ve} + \frac{1}{2} L_{mnn}^{(2)} \bar{\zeta}_m \bar{\zeta}_n + a_1(\bar{\epsilon}^{ve}) L_{ijn}^{(3)} \bar{\epsilon}_{ij}^{ve} \bar{\zeta}_n \right] \vartheta^{ve} \quad (87)$$

where $a_0(\bar{\epsilon}^{ve})$ and $a_1(\bar{\epsilon}^{ve})$ are nonlinear dependency scalars which are introduced in the Helmholtz free energy to make the viscoelastic model nonlinear (Schapery, 1969b). These parameters are functions of the viscoelastic strain tensor. The matrices $L^{(1)}$, $L^{(2)}$, and $L^{(3)}$ are positive definite. The parameter ϑ^{ve} in Eq. (87) can be an Arrhenius-type temperature term for coupling temperature to the viscoelastic constitutive law and is defined as follows:

$$\vartheta^{ve} = \exp \left[-\theta_1 \left(1 - \frac{T}{T_0} \right) \right] \quad (88)$$

where θ_1 is a material parameter and T_0 is the reference temperature.

The energetic component of the stress can be easily derived using Eqs. (56) and (87), such that:

$$\bar{\sigma}_{ij}^{ene} = \left(A_{ijtu}^{(0)} L_{tukl}^{(1)} \bar{\epsilon}_{kl}^{ve} + A_{ijtu}^{(1)} L_{tun}^{(3)} \bar{\zeta}_n \right) \vartheta^{ve} \quad (89)$$

where $A_{ijtu}^{(0)}$ and $A_{ijtu}^{(1)}$ are nonlinear parameters related to the instantaneous and transient viscoelastic responses, respectively. Eq. (89) shows that the instantaneous nonlinear parameters are no longer scalars for 3D models and are defined as follows:

$$A_{ijtu}^{(0)} = a_0 \delta_{it} \delta_{ju} + \frac{1}{2} \frac{\partial a_0}{\partial \bar{\epsilon}_{ij}^{ve}} \bar{\epsilon}_{tu}^{ve}; \quad A_{ijtu}^{(1)} = a_1 \delta_{it} \delta_{ju} + \frac{\partial a_1}{\partial \bar{\epsilon}_{ij}^{ve}} \bar{\epsilon}_{tu}^{ve} \quad (90)$$

Eq. (89) also shows that the energetic component of the stress has two terms, one of which is related to instantaneous response and the other one is related to the recoverable processes associated with the viscoelastic internal state variables. These two terms are recovered upon the unloading and no energy dissipates due to these terms. However, the dissipation mechanism results from the viscoelastic strain rate and the rate of the viscoelastic internal state variables which are related to the chain mobility and friction between the polymer chains. In this work, we postulate the following simple quadratic form for the viscoelastic component of the rate of energy dissipation:

$$\Pi^{tve} = [\mu_{ijkl} \dot{\bar{\epsilon}}_{ij}^{ve} \dot{\bar{\epsilon}}_{kl}^{ve} + P_{mn} \dot{\bar{\zeta}}_m \dot{\bar{\zeta}}_n] \vartheta^{ve} \tag{91}$$

Parameters in Eq. (91) are defined as follows:

$$\mu_{ijkl} = \frac{1}{\vartheta^{ve}} \frac{\partial \Pi^{tve}}{\partial \dot{\bar{\epsilon}}_{ij}^{ve} \partial \dot{\bar{\epsilon}}_{kl}^{ve}}; \quad P_{mn} = \frac{1}{\vartheta^{ve}} \frac{\partial \Pi^{tve}}{\partial \dot{\bar{\zeta}}_m \partial \dot{\bar{\zeta}}_n} \tag{92}$$

The same Arrhenius-type temperature coupling terms are assumed for both the temperature-dependent Helmholtz free energy and rate of energy dissipation. Moreover, note that the assumed form for the thermo-viscoelastic component of rate of energy dissipation guarantees the rate of the energy dissipation to be always positive. Another common assumption in the theory of nonlinear viscoelasticity is that the thermodynamic conjugate forces can be expressed as a nonlinear function of the evolution of the state variables (see e.g. [Schapery, 1969a](#); [Levesque et al., 2008](#)). Here, we show that there is no need to make these assumptions and the viscoelastic laws can be derived directly from the viscoelastic microforce balance (Eq. (39)). The viscoelastic microforce balance indicates that the summation of the energetic and dissipative components of the thermodynamic forces $\bar{\chi}_n$ conjugate to the viscoelastic internal state variables $\bar{\zeta}_n$ is zero, such that:

$$\bar{\chi}_n = 0 \Rightarrow \bar{\chi}_n^{ene} + \bar{\chi}_n^{dis} = 0 \tag{93}$$

The energetic and dissipative components of the viscoelastic conjugate forces can be determined using Eqs. (50)₂, (80)₂, (87), and (91), such that:

$$\bar{\chi}_n^{ene} = [L_{mn}^{(2)} \bar{\zeta}_m + a_1 (\bar{\epsilon}^{ve}) L_{ijn}^{(3)} \bar{\epsilon}_{ij}^{ve}] \vartheta^{ve}; \quad \bar{\chi}_n^{dis} = (P_{mn} \dot{\bar{\zeta}}_m) \vartheta^{ve} \tag{94}$$

Substituting Eq. (94) into Eq. (93) yields:

$$P_{mn} \dot{\bar{\zeta}}_m + L_{mn}^{(2)} \bar{\zeta}_m + a_1 (\bar{\epsilon}^{ve}) L_{ijn}^{(3)} \bar{\epsilon}_{ij}^{ve} = 0 \tag{95}$$

Eq. (95) is the partial differential equation governing the viscoelastic processes. This equation relates the viscoelastic internal state variables $\bar{\zeta}_n$ to the viscoelastic strain tensor $\bar{\epsilon}^{ve}$. Furthermore, Eq. (95) represents a coupled system of differential equations that express the evolution of $\bar{\zeta}_n$ as a function of $\bar{\epsilon}_{ij}^{ve}$. Since \mathbf{P} , $\mathbf{L}^{(2)}$, and $\mathbf{L}^{(3)}$ are positive definite, it is always possible to find a basis in which these tensors are diagonal ([Levesque et al., 2008](#)). Suppose for simplicity that these tensors are already expressed in this basis. Then Eq. (95) becomes:

$$P_{mm} \dot{\bar{\zeta}}_m + L_{mm}^{(2)} \bar{\zeta}_m + a_1 (\bar{\epsilon}^{ve}) L_{ijm}^{(3)} \bar{\epsilon}_{ij}^{ve} = 0; \quad (\text{No sum on } m) \tag{96}$$

Using the Laplace transform one can write:

$$\bar{\zeta}_m(\psi) = -\frac{L_{ijm}^{(3)}}{L_{mm}^{(2)}} \int_0^t (1 - \exp[-\omega_m(t - \tau)]) \frac{d}{d\tau} (a_1 \bar{\epsilon}_{ij}^{ve}) d\tau; \quad (\text{No sum on } n) \tag{97}$$

where $\omega_m = \frac{L_{mm}^{(2)}}{P_{mm}}$.

Eq. (97) shows the relation between $\bar{\zeta}_m$ and $\bar{\epsilon}_{ij}^{ve}$. It is clear from Eq. (97) that $\bar{\zeta}_m$ depends also on the viscoelastic deformation history; hence, $\bar{\zeta}_m$ evolves with the evolution of $\bar{\epsilon}_{ij}^{ve}$. This supports our argument of decomposing the total stress into energetic and dissipative components. Also, Eq. (97) shows that assuming $\bar{\zeta}_m$ to be constant (i.e. $\dot{\bar{\zeta}}_m = 0$) is valid only when $\bar{\epsilon}_{ij}^{ve}$ is constant (i.e. $\dot{\bar{\epsilon}}_{ij}^{ve} = 0$), which occurs only in the absence of the viscoelastic processes. Hence, it is not consistent to make this argument to derive a viscoelasticity law as presented by several researchers ([Levesque et al., 2008](#)).

Now, we can simply obtain the dissipative component of the stress using Eqs. (80) and (91), such that:

$$\bar{\sigma}_{ij}^{dis} = \mu_{ijkl} \dot{\bar{\epsilon}}_{kl}^{ve} \tag{98}$$

The stress as a function of $\bar{\epsilon}_{ij}^{ve}$ can now be obtained by substituting Eqs. (89), (97), and (98) into Eq. (56), such that:

$$\bar{\sigma}_{ij} = \mu_{ijkl} \dot{\bar{\epsilon}}_{kl}^{ve} + G_{ijtu}^{(0)} E_{tukl}^{(0)} \vartheta^{ve} \bar{\epsilon}_{kl}^{ve} + G_{ijtu}^{(1)} \vartheta^{ve} \int_0^t \left[\sum_{m=1}^M E_{tukl}^{(m)} (1 - \exp[-\omega_m(t - \tau)]) \right] \frac{d(g^{(2)} \bar{\epsilon}_{kl}^{ve})}{d\tau} d\tau \tag{99}$$

where

$$G_{ijtu}^{(0)} E_{tukl}^{(0)} = A_{ijtu}^{(0)} L_{tukl}^{(1)} - a_1 A_{ijtu}^{(1)} \frac{L_{tum}^{(3)} L_{klm}^{(3)}}{L_{mm}^{(2)}} \tag{100}$$

$$G_{ijtu}^{(1)} = A_{ijtu}^{(1)}; \quad E_{tukl}^{(m)} = \frac{L_{tum}^{(3)} L_{klm}^{(3)}}{L_{mm}^{(2)}}; \quad g^{(2)} = a_1 \tag{101}$$

Eq. (99) represents a more comprehensive formulation that relates the total stress to the viscoelastic strain comparing to [Levesque et al. \(2008\)](#). According to notations of [Duvaut and Lions \(1976\)](#), the first two terms in the right hand side of Eq. (99) refers to viscoelastic materials with short memories since these two terms relate the state of stress at time t only

to the strains at current time t and immediately preceding t . However, the third term in the right hand side of Eq. (99) corresponds to viscoelastic materials with long term memory since it relates the state stress at t to strains at the times preceding t . For the case of linear viscoelasticity the nonlinear parameters should be always unity (i.e. $\mathbf{G}^{(0)} = \mathbf{G}^{(1)} = \mathbf{I}$ and $g^{(2)} = 1$) which simplifies Eq. (99), such that:

$$\bar{\sigma}_{ij} = \mu_{ijkl} \dot{\bar{\epsilon}}_{kl}^{ve} + E_{ijkl}^{(0)} \vartheta^{ve} \bar{\epsilon}_{kl}^{ve} + \vartheta^{ve} \int_0^t \left[\sum_{m=1}^M E_{ijkl}^{(m)} (1 - \exp[-\omega_m(t - \tau)]) \right] \frac{d\bar{\epsilon}_{kl}^{ve}}{d\tau} d\tau \quad (102)$$

Eq. (102) shows the simple viscoelastic constitutive model for linear viscoelastic materials.

Moreover, the last two terms in the right-hand-side of Eq. (99) can be considered as the general form of the 3D Schapery-type viscoelastic model. Eq. (99) shows that the nonlinear parameter $g^{(2)}$ can still remain a scalar for 3D viscoelastic models. However, the instantaneous nonlinear parameter $\mathbf{G}^{(0)}$ and the transient nonlinear parameter $\mathbf{G}^{(1)}$ should be tensors for general Schapery-type 3D viscoelastic models. Also, we clearly see that the temperature-dependency can easily be incorporated into the viscoelastic models using a temperature coupling term for all terms in the right-hand-side of Eq. (99). This approach is more general comparing to the classical Schapery-type viscoelasticity where the temperature-shift factor is introduced in the definition of reduced time (Schapery, 1969b). The reason is that the incorporation of the temperature-shift factor as part of the reduced time variable only makes the third term in Eq. (99) temperature-dependent. However, using the proposed temperature coupling term makes all terms of Eq. (99) to depend on temperature. Moreover, as it was mentioned earlier, two temperature coupling terms can be introduced in Eq. (99), one is related to Helmholtz free energy affecting the instantaneous response and the other is related to the rate of energy dissipation affecting the rate-type and the transient responses. Furthermore, using ϑ^{ve} implies that the nonlinear parameters $\mathbf{G}^{(0)}$, $\mathbf{G}^{(1)}$, and $g^{(2)}$ are identified at a reference temperature which makes their calibration easier. It is noteworthy that a proper viscoelastic model can be derived for a specific material by postulating different mathematical forms for viscoelastic components of Helmholtz free energy and rate of energy dissipation.

The relation for obtaining the viscoelastic strain as a function of the stress can also be determined by using the Laplace transform. Schapery (1969b) used the thermodynamic of irreversible processes based on Gibbs free energy to derive the relationship for the viscoelastic strain as a function of the stress. His formulation for nonlinear viscoelasticity can be expressed as the following in the healing configuration:

$$\bar{\epsilon}_{ij}^{ve} = g_0 C_{ijkl}^{(0)} \bar{\sigma}_{kl} + g_1 \int_0^\psi \sum C_{ijkl}^m \exp[-\omega_m(\psi - \psi^\tau)] \frac{d(g_2 \bar{\sigma}_{kl})}{d\tau} d\tau \quad (103)$$

where \mathbf{C} is a fourth-order tensor representing the creep compliance tensor.

4.2. Thermo-viscoplasticity flow rule

In this section, we show how to derive the generalized non-associative viscoplasticity yield conditions and potential functions based on the viscoplastic microforce balance, Eq. (27), and the relationship between the yield surface and plastic potential derived based on the principle of virtual power [as presented in Appendix A, Eqs. (A.16) and (A.17)]. However, since we will couple viscoelasticity and viscoplasticity to damage and micro-damage healing, we express the viscoplastic constitutive model in the healing configuration. Both isotropic and kinematic hardenings are considered. Also, an evolution equation similar to Armstrong and Frederick model (1966) is derived using the presented framework.

As shown in Section 3.3, the non-associative viscoplasticity can be derived based on the principle of virtual power. Eq. (A.16) represents the relationship between the yield surface and the plastic potential function. Hence, we can derive the thermodynamically consistent viscoplastic potential associated with a given viscoplasticity yield surface or vice versa. In this section, we derive the thermodynamically consistent dynamic yield surface associated with a given viscoplastic potential function. Eq. (A.16) naturally yields non-associative viscoplasticity for a given viscoplastic potential. We use the normality rule for non-associative plasticity in the healing configuration which states that the direction of the rate of viscoplastic strain tensor in the healing configuration is normal to the viscoplastic potential function. Hence, there exists a viscoplastic potential function for which the direction of the viscoplastic flow in the healing configuration, $\bar{\mathbf{N}}$, in Eq. (A.14) and can be defined as follows:

$$\bar{\mathbf{N}}_{ij} = \frac{\partial \bar{F}}{\partial (\bar{\sigma}_{ij} - \bar{X}_{ij})} \quad (104)$$

where \bar{F} is the viscoplastic potential function. Comparing Eqs. (40) and (104) implies:

$$\dot{\bar{\epsilon}}_{ij}^{vp} = \sqrt{\frac{3}{2}} \dot{\bar{p}} \bar{\mathbf{N}}_{ij} = \sqrt{\frac{3}{2}} \dot{\bar{p}} \frac{\partial \bar{F}}{\partial (\bar{\sigma}_{ij} - \bar{X}_{ij})} \quad (105)$$

We postulate a modified Drucker–Prager-type viscoplastic potential function to make the viscoplasticity model able to capture the effect of confinement and multi-axial state of the stress, such that:

$$\bar{F} = \bar{\tau}^{vp} - \alpha \bar{I}_1 \quad (106)$$

where $\bar{\tau}^{vp}$ is the equivalent shear stress in the healing configuration modified to distinguish between different viscoplastic responses of materials under contraction and extension loading conditions, which can be defined as follows (Abu Al-Rub et al., 2010):

$$\bar{\tau}^{vp} = \frac{\sqrt{3\bar{J}_2}}{2} \left[1 + \frac{1}{d^{vp}} + \left(1 - \frac{1}{d^{vp}} \right) \frac{3\bar{J}_3}{\sqrt{3\bar{J}_2^3}} \right] \tag{107}$$

where \bar{I}_1 is the first stress invariant, \bar{J}_2 is the second invariant of the deviatoric stress, and \bar{J}_3 is the third invariant of the deviatoric stress defined as:

$$\bar{I}_1 = \frac{1}{3} \bar{\sigma}_{kk}; \quad \bar{J}_2 = \frac{1}{2} (\bar{S}_{ij} - \bar{X}_{ij})(\bar{S}_{ij} - \bar{X}_{ij}); \quad \bar{J}_3 = \frac{1}{2} (\bar{S}_{ij} - \bar{X}_{ij})(\bar{S}_{jk} - \bar{X}_{jk})(\bar{S}_{ki} - \bar{X}_{ki}) \tag{108}$$

where \bar{S} is the deviatoric part of the Cauchy stress tensor in the healing configuration $\bar{\sigma}$ (i.e. $\bar{S}_{ij} = \bar{\sigma}_{ij} - \frac{1}{3} \bar{\sigma}_{kk} \delta_{ij}$).

Fig. 3 shows the plastic potential surface in 3D principal stress space for different values of d^{vp} parameter. As it is clear from Fig. 3, d^{vp} in Eq. (107) is a material parameter which is interpreted as the ratio of the yield stress in the uniaxial tension to that in the uniaxial compression. Therefore, d^{vp} gives the distinction of the material response in compressive and tensile loading conditions.

Eq. (107) has been used as the modified Drucker–Prager plasticity by several researchers (Drucker et al., 1957; Chen and Mizuno, 1990; Dessouky, 2005; Han et al., 2008), but expressed in the damaged (nominal) configuration. In this work, this viscoplastic potential function is used since it has been successfully applied to pressure sensitive materials in several cases (Dessouky, 2005; Masad et al., 2005; Abu Al-Rub et al., 2010; Darabi et al., 2011a). Using Eqs. (104), (106), and (107) yields:

$$\bar{N}_{ij} = \frac{\sqrt{3}}{4} \left(1 + \frac{1}{d^{vp}} \right) \frac{(\bar{S}_{ij} - \bar{X}_{ij})}{\sqrt{\bar{J}_2}} + \left(1 - \frac{1}{d^{vp}} \right) \frac{1}{\bar{J}_2} \left[\frac{9}{4} \bar{J}_2 (\bar{S}_{ik} - \bar{X}_{ik})(\bar{S}_{kj} - \bar{X}_{kj}) - \frac{3}{2} \bar{J}_3 (\bar{S}_{ij} - \bar{X}_{ij}) \right] - \left[\frac{3}{2} \left(1 - \frac{1}{d^{vp}} \right) + \frac{\alpha}{3} \right] \delta_{ij} \tag{109}$$

Substituting Eq. (109) into the viscoplastic microforce balance (Eq. (A.16)) yields:

$$f = \bar{\tau}^{vp} - \beta \bar{I}_1 - \sqrt{\frac{2}{3}} \bar{R} = 0 \tag{110}$$

where $\beta = \alpha + \frac{9}{2} \left(1 - \frac{1}{d^{vp}} \right)$. Eq. (110) shows the expression of the yield surface associated with the assumed viscoplastic potential function in Eq. (106). Comparing Eqs. (106) and (110) clearly shows that assuming a Drucker–Prager-type viscoplastic potential function yields a non-associative viscoplasticity theory where the yield surface and viscoplastic potential are different.

It should be mentioned that one of the common ways to obtain viscoplasticity theories is to treat Eq. (110) as the rate-independent plasticity yield surface and extend it to rate-dependent plasticity (viscoplasticity) using the overstress concept (Zener and Hollomon, 1944; Malvern, 1951; Perzyna, 1986; Perzyna and Korbel, 1998). According to this approach, the extension of the plasticity yield surface to the rate-dependent plasticity (viscoplasticity) theory is usually accompanied

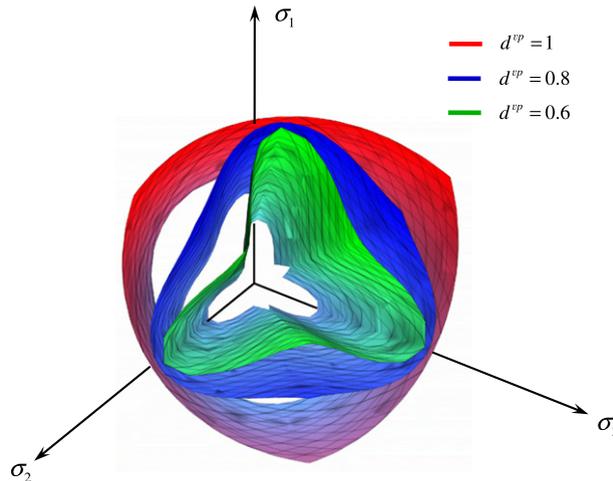


Fig. 3. The viscoplastic potential function for different values of d^{vp} in 3D space of principal stresses. d^{vp} captures the multi-axial effect of the stress and distinguishes between the extension and contraction loading conditions. It should be noted that d^{vp} should range between 0.78 and 1 to ensure the convexity of the viscoplasticity yield surface.

by the assumption that the stress state is no longer on the yield surface. Hence, an overstress function is defined in a dynamic yield surface to constrain the stress state to remain on the dynamic yield surface. Then by defining an admissible form of the plasticity Lagrange multiplier as a function of the overstress, the dynamic yield surface can be obtained (see Voyiadjis et al., 2004 for more details). However, we will show here that there is no need for extending Eq. (110) to viscoplasticity. In other words, the viscoplasticity dynamic yield surface obtains directly from Eq. (110) if the hardening conjugate force \bar{R} is properly decomposed into energetic and dissipative components, Eq. (57)₂ (i.e. $\bar{R} = \bar{R}^{\text{ene}} + \bar{R}^{\text{dis}}$). The next step is to postulate mathematical forms for the thermo-viscoplastic component of the Helmholtz free energy, Ψ^{tvp} , and the rate of thermo-viscoplastic energy dissipation, Π^{tvp} , in order to define the dynamic yield surface for the assumed viscoplastic potential. Here, the following positive definite forms are postulated for Ψ^{tvp} and Π^{tvp} , respectively,

$$\rho \Psi^{\text{tvp}} = \left[\frac{1}{2} C_1 \bar{\epsilon}_{ij}^{\text{vp}} \bar{\epsilon}_{ij}^{\text{vp}} + \kappa_0 \bar{p} + \kappa_1 \left(\bar{p} + \frac{1}{\kappa_2} \exp(-\kappa_2 \bar{p}) \right) \right] \vartheta^{\text{vp}} \quad (111)$$

$$\Pi^{\text{tvp}} = \left[C_2 \exp(-\gamma \bar{p}) \dot{\bar{\epsilon}}_{ij}^{\text{vp}} \dot{\bar{\epsilon}}_{ij}^{\text{vp}} + C_3 \Gamma^{\text{vp}} \left(\frac{\dot{\bar{p}}}{\Gamma^{\text{vp}} \vartheta^{\text{vp}}} \right)^{1+\frac{1}{N}} \right] \vartheta^{\text{vp}} \quad (112)$$

where κ_0 , κ_1 , κ_2 , C_1 , C_2 , C_3 , and N are material parameters; and Γ^{vp} is another material parameter representing the viscoplasticity fluidity parameter. The parameter ϑ^{vp} is another Arrhenius-type temperature term for coupling temperature to the viscoplastic constitutive equations and is defined as follows:

$$\vartheta^{\text{vp}} = \exp \left[-\theta_2 \left(1 - \frac{T}{T_0} \right) \right] \quad (113)$$

where θ_2 is the viscoplastic temperature coupling term parameter. It is noteworthy that for certain materials such as bituminous and polymeric materials viscoelastic and viscoplastic temperature coupling terms can be assumed to be the same (i.e. $\vartheta^{\text{ve}} = \vartheta^{\text{vp}}$) (Schwartz et al., 2002).

Now, the energetic components of the isotropic and kinematic hardening conjugate forces can be determined by substituting Eq. (111) into Eq. (51), such that:

$$\bar{R}^{\text{ene}} = [\kappa_0 + \kappa_1 (1 - \exp(-\kappa_2 \bar{p}))] \vartheta^{\text{vp}}; \quad \bar{X}_{ij}^{\text{ene}} = C_1 \bar{\epsilon}_{ij}^{\text{vp}} \vartheta^{\text{vp}} \quad (114)$$

The dissipative components of the isotropic and kinematic hardening conjugate forces are also determined by substituting Eq. (112) into Eq. (81), such that:

$$\bar{R}^{\text{dis}} = C_3 \left(\frac{\dot{\bar{p}}}{\Gamma^{\text{vp}} \vartheta^{\text{vp}}} \right)^{\frac{1}{N}}; \quad \bar{X}_{ij}^{\text{dis}} = C_2 \exp(-\gamma \bar{p}) \dot{\bar{\epsilon}}_{ij}^{\text{vp}} \vartheta^{\text{vp}} \quad (115)$$

Hence, the total isotropic hardening function, $\bar{R} = \bar{R}^{\text{ene}} + \bar{R}^{\text{dis}}$, and the total kinematic hardening function, $\bar{X}_{ij} = \bar{X}_{ij}^{\text{ene}} + \bar{X}_{ij}^{\text{dis}}$, can be written as follows:

$$\bar{R} = [\kappa_0 + \kappa_1 (1 - \exp(-\kappa_2 \bar{p}))] \vartheta^{\text{vp}} + C_3 \left(\frac{\dot{\bar{p}}}{\Gamma^{\text{vp}} \vartheta^{\text{vp}}} \right)^{\frac{1}{N}} \quad (116)$$

$$\bar{X}_{ij} = [C_1 \bar{\epsilon}_{ij}^{\text{vp}} + C_2 \exp(-\gamma \bar{p}) \dot{\bar{\epsilon}}_{ij}^{\text{vp}}] \vartheta^{\text{vp}} \quad (117)$$

The dynamic viscoplastic yield surface can now be determined by substituting Eqs. (116) and (117) into Eq. (110), such that:

$$\bar{\tau}^{\text{vp}} - \beta \bar{I}_1 - \sqrt{2/3} [\kappa_0 + \kappa_1 (1 - \exp(-\kappa_2 \bar{p}))] \vartheta^{\text{vp}} - \sqrt{2/3} C_3 \left(\frac{\dot{\bar{p}}}{\Gamma^{\text{vp}} \vartheta^{\text{vp}}} \right)^{\frac{1}{N}} = 0 \quad (118)$$

Eq. (118) represents the temperature-dependent dynamic yield surface associated with the assumed viscoplastic potential function in Eq. (106). Rearranging Eq. (118) for $\dot{\bar{p}}$ gives:

$$\dot{\bar{p}} = \Gamma^{\text{vp}} \vartheta^{\text{vp}} \left\langle \frac{\bar{\tau}^{\text{vp}} - \beta \bar{I}_1 - [\kappa_0 + \kappa_1 (1 - \exp(-\kappa_2 \bar{p}))] \sqrt{2/3} \vartheta^{\text{vp}}}{C_3 \sqrt{2/3}} \right\rangle^N \quad (119)$$

Substituting Eq. (119) into Eq. (105) yields the following Perzyna-type non-associated thermo-viscoplasticity flow rule, such that:

$$\dot{\bar{\epsilon}}_{ij}^{\text{vp}} = \Gamma^{\text{vp}} \vartheta^{\text{vp}} \left\langle \frac{\bar{\tau}^{\text{vp}} - \beta \bar{I}_1 - [\kappa_0 + \kappa_1 (1 - \exp(-\kappa_2 \bar{p}))] \sqrt{2/3} \vartheta^{\text{vp}}}{C_3 \sqrt{2/3}} \right\rangle^N \bar{N}_{ij} \quad (120)$$

where $\bar{N}_{ij} = \frac{\partial \bar{F}}{\partial (\sigma_{ij} - \bar{X}_{ij})}$. We can also assume $C_3 = \bar{R}^{\text{ene}}$ in the above equation or in Eq. (112), which assumes C_3 to be dependent on the equivalent viscoplastic strain \bar{p} as in Eq. (114).

Taking the time derivative of Eqs. (114)₂ and (115)₂ at fixed temperature give:

$$\dot{\bar{X}}_{ij}^{\text{ene}} = C_1 \dot{\bar{\epsilon}}_{ij}^{\text{vp}} \vartheta^{\text{vp}}; \quad \dot{\bar{X}}_{ij}^{\text{dis}} = \left[-\gamma C_2 \dot{\bar{p}} \exp(-\gamma \bar{p}) \dot{\bar{\epsilon}}_{ij}^{\text{vp}} + C_2 \exp(-\gamma \bar{p}) \ddot{\bar{\epsilon}}_{ij}^{\text{vp}} \right] \vartheta^{\text{vp}} \quad (121)$$

Adding both sides of Eq. (121)₁ and (121)₂; and making use of Eqs. (114)₂ and (115)₂ yield the following evolution equation for the backstress:

$$\dot{\bar{X}}_{ij} = \left[C_1 \dot{\bar{\epsilon}}_{ij}^{\text{vp}} - \gamma \dot{\bar{p}} \bar{X}_{ij}^{\text{dis}} + C_2 \exp(-\gamma \bar{p}) \ddot{\bar{\epsilon}}_{ij}^{\text{vp}} \right] \vartheta^{\text{vp}} \quad (122)$$

Eq. (122) shows the equation for the evolution of the backstress. This equation can be considered as the modified Armstrong–Frederick model (Armstrong and Frederick, 1966). When the loading rate is not too high, the effect of $\ddot{\bar{\epsilon}}_{ij}^{\text{vp}}$ can be neglected. In this case Eq. (122) reduces to at reference temperature:

$$\dot{\bar{X}}_{ij} = C_1 \dot{\bar{\epsilon}}_{ij}^{\text{vp}} - \gamma \dot{\bar{p}} \bar{X}_{ij}^{\text{dis}} \quad (123)$$

The Armstrong–Frederick model for evolution of backstress is written as follows in the healing configuration:

$$\dot{\bar{X}}_{ij} = C_1 \dot{\bar{\epsilon}}_{ij}^{\text{vp}} - \gamma \dot{\bar{p}} \bar{X}_{ij} \quad (124)$$

Eqs. (123) and (124) are similar except that the total backstress tensor in the right-hand-side of Eq. (124) is replaced by its dissipative component in Eq. (123). Also, Eq. (123) yields the linear kinematic hardening rule when $\gamma = 0$ (Prager, 1956). Eq. (123) can also be rewritten in the following form:

$$\dot{\bar{X}}_{ij} = C_1 \dot{\bar{\epsilon}}_{ij}^{\text{vp}} - \gamma \dot{\bar{p}} \bar{X}_{ij} + \gamma \dot{\bar{p}} \bar{X}_{ij}^{\text{ene}} \quad (125)$$

The first two terms represent the Armstrong–Frederick model in the healing configuration. However, Eq. (125) shows that the energetic component of the kinematic hardening function is missing in the Armstrong–Frederick model.

The presented overstress viscoplasticity model, Eq. (120), will be used in the second part of this paper to predict the response of bituminous materials at low and intermediate loading rates (Darabi et al., submitted for publication). However, as argued by Hashiguchi et al. (2005), the model cannot be effectively applied to predict the deformation response at infinite rates of loading. In other words, within the practical range of the model parameter N (Eq. (120)), the stress increases almost elastically at an infinite rate of deformation (e.g. impact loading). To overcome this issue Hashiguchi (2009) modified the overstress model by incorporating another model parameter designating the maximum ratio of the yield function over the hardening function, such that Eq. (120) can be modified as:

$$\dot{\bar{\epsilon}}_{ij}^{\text{vp}} = \Gamma^{\text{vp}} \vartheta^{\text{vp}} \frac{(\bar{\tau}^{\text{vp}} - \beta \bar{I}_1 - R(\bar{p}))}{f_m R(\bar{p}) - (\bar{\tau}^{\text{vp}} - \beta \bar{I}_1)} \bar{N}_{ij} \quad (126)$$

where f_m is a model parameter designating the maximum value of the ratio $f_m = (\bar{\tau}^{\text{vp}} - \beta \bar{I}_1)/R(\bar{p})$; where $f_m \approx 1$ is usually assumed (Hashiguchi et al., 2005; Hashiguchi, 2009).

These examples show the capabilities of the proposed thermodynamic framework in deriving different constitutive models for different types of materials. In the next sections, we apply the presented framework in deriving viscodamage and micro-damage healing loading conditions and evolution laws.

4.3. Viscodamage constitutive equations

In classical continuum damage mechanics a damage condition is usually postulated to determine the onset of damage growth and evolution (Hayakawa and Murakami, 1997; Murakami et al., 1998). This damage function is treated very similar to plasticity theory. As a result, the extension of the damage condition to the rate-dependent one is also carried out similarly to the extension of rate-independent plasticity yield surface to the dynamic viscoplasticity yield surface (Voyiadjis et al., 2004). However, here we will show that the rate-dependent damage (viscodamage) condition can be derived directly from the principle of virtual power and laws of thermodynamics. Eq. (28) defines the damage microforce balance. It will be shown here that this microforce balance is in fact the damage growth condition. Combining Eq. (28) with Eq. (58) yields:

$$Y = 0 \Rightarrow Y^{\text{ene}} + Y^{\text{dis}} = 0 \Rightarrow Y^{\text{ene}} = -Y^{\text{dis}} \quad (127)$$

where Y^{ene} and Y^{dis} are given in Eqs. (52) and (82), respectively. To the best of the authors' knowledge, this interesting result has been reported here for the first time. In fact, Eq. (127) is the damage condition criterion. Based on the mathematical form of thermo-viscodamage Helmholtz free energy, Ψ^{tvd} , and rate of thermo-viscodamage energy dissipation, Π^{tvd} , the damage condition can be rate-independent or rate-dependent. Wu et al. (2006) proposed an energy-based plastic-damage model for concrete in which the Helmholtz free energy in the presence of damage is expressed as a function of stress invariants and damage variable. Similar assumptions have been made by Voyiadjis et al. (2004), Voyiadjis and Abu Al-Rub (2006), and Abu Al-Rub and Kim (2009). Therefore, the following form is postulated for the thermo-viscodamage component of the Helmholtz free energy to consider the confinement effects, the different effects of damage in tensile and compressive loading conditions, and the effect of temperature on damage evolution and growth, such that:

$$\rho \Psi^{tvd} = \frac{1}{b_1} (1 - \phi)^{b_1} \left[\frac{\bar{\tau}^{vd} - \alpha \bar{I}_1}{b_2} \right] \exp(b_3 \bar{\varepsilon}_{eff}) \vartheta^{vd} \quad (128)$$

where b_1 , b_2 , and b_3 are material parameters. Note that when $\phi = 0$ (i.e. no damage) the damage component of the Helmholtz free energy has its initial value. However, when the damage variable increases and material becomes more damaged, the free energy function due to the damage decreases and eventually reaches zero at complete failure (i.e. $\phi = 1$). Also, the damage component of the Helmholtz free energy is assumed to be a function of the total effective strain in the healing configuration (i.e. $\bar{\varepsilon}_{eff} = \sqrt{\bar{\varepsilon}_{ij} \bar{\varepsilon}_{ij}}$) to enhance more couplings between viscoelasticity, viscoplasticity, and viscodamage. The equivalent shear stress $\bar{\tau}^{vd}$ in Eq. (128) is defined similar to Eq. (107) for viscoplasticity, such that:

$$\bar{\tau}^{vd} = \frac{\sqrt{3J_2}}{2} \left[1 + \frac{1}{d^{vd}} + \left(1 - \frac{1}{d^{vd}} \right) \frac{3\bar{J}_3}{\sqrt{3J_2^3}} \right] \quad (129)$$

where d^{vd} is a material parameter distinguishing different damage responses in tension and compression loading conditions and can be defined as the ratio of the damage threshold force in uniaxial tension to that in the uniaxial compression. The parameter ϑ^{vd} in Eq. (128) is another Arrhenius-type temperature coupling term for making the viscodamage law temperature-dependent and is defined as follows:

$$\vartheta^{vd} = \exp \left[-\theta_3 \left(1 - \frac{T}{T_0} \right) \right] \quad (130)$$

where θ_3 is viscoplastic temperature coupling term parameter.

The energetic component of the viscodamage force Y^{ene} can now be determined by substituting Eq. (128) into Eq. (52), such that:

$$Y^{ene} = -(1 - \phi)^{b_1 - 1} \left[\frac{\bar{\tau}^{vd} - \alpha \bar{I}_1}{b_2} \right] \exp(b_3 \bar{\varepsilon}_{eff}) \vartheta^{vd} \quad (131)$$

An expression similar to that assumed for the second part of the thermo-viscoplastic rate of energy dissipation, Eq. (112), is postulated for the rate of the thermo-viscodamage energy dissipation, Π^{tvd} , such that:

$$\Pi^{tvd} = b_0 \Gamma^{vd} \left(\frac{\dot{\phi}}{\Gamma^{vd} \vartheta^{vd}} \right)^{1 + \frac{1}{q}} \quad (132)$$

here b_0 and q are material constants, and Γ^{vd} is the viscodamage fluidity parameter which controls the rate of damage evolution. Moreover, b_0 can be assumed to be dependent on $-Y^{ene}$, as argued for viscoplasticity, for more general damage evolution equations. Then, the dissipative component of the damage thermodynamic force, Y^{dis} , can be obtained by substituting Eq. (132) into Eq. (82), which yields:

$$Y^{dis} = b_0 \Gamma^{vd} \vartheta^{vd} \left(\frac{\dot{\phi}}{\Gamma^{vd} \vartheta^{vd}} \right)^{1 + \frac{1}{q}} \quad (133)$$

with $\hat{\lambda}^{vd} = (1 + 1/q)^{-1}$. Now, we can obtain the rate-dependent damage surface by substituting Eqs. (131) and (133) into Eq. (127) that results in the following equation:

$$(1 - \phi)^{b_1 - 1} \left[\frac{\bar{\tau} - \alpha \bar{I}_1}{b_2} \right] \exp(b_3 \bar{\varepsilon}_{eff}) \vartheta^{vd} - b_0 \left(\frac{\dot{\phi}}{\Gamma^{vd} \vartheta^{vd}} \right)^{\frac{1}{q}} = 0 \quad (134)$$

Eq. (134) represents the dynamic viscodamage loading condition for temperature- and rate-dependent damage (thermo-viscodamage). This equation can also be represented as a damage evolution law, such that:

$$\dot{\phi} = \Gamma^{vd} \left[\frac{(1 - \phi)^{b_1 - 1} (\bar{\tau} - \alpha \bar{I}_1)}{b_2 b_0} \right]^q \exp(b_3 q \bar{\varepsilon}_{eff}) \hat{\vartheta}^{vd} \quad (135)$$

where $\hat{\vartheta}^{vd} = (\vartheta^{vd})^{1 + \frac{1}{q}}$. It is noteworthy to mention that Darabi et al. (2011a) successfully applied and validated a simplified version of Eq. (135) to predict the rate-dependent damage response of bituminous materials. The proposed framework presented in this section can be generalized to anisotropic damage which will be the focus of a future work.

4.4. Micro-damage healing constitutive equations

As it was mentioned in the Introduction, some engineering materials have the potential to heal and retrieve part of their strength and stiffness during the rest period (i.e. the external loading is removed from the body). During the rest period some

micro-crack and micro-void free surfaces wet and are brought back into contact with one another. In certain materials such as polymers and especially bituminous materials, micro-cracks and micro-voids gradually reduce in size with a corresponding recovery in strength and stiffness (Wool and Oconnor, 1981). This process is referred to as *micro-damage healing*. The micro-damage healing process can be described as a combination of a short term healing (wetting) and long term healing (intrinsic healing) (e.g. de Gennes, 1971; Wool and Oconnor, 1981; Bhasin et al., 2011). During the short term healing, crack surfaces wet and coming into contact with each other. Due to the surface free energy of the crack faces, partial bonding occurs almost instantaneously which leads to partial strength and stiffness recovery at the macro-scale. Once the crack surfaces wet each other, the intrinsic healing continues over time due to the self diffusion of molecules across the crack interface. The driving force for this self-diffusion is triggered by the sharp decrease in the bulk density of the material near the cracked area. The created density gradient is the driving force for the self-diffusion of some molecules to low density region which is around the crack faces. The rate of self-diffusion of molecules across the crack interfaces depends on the chemical structure and size of the molecules which controls the rate of long term micro-damage healing and subsequently strength and stiffness recovery. Hence, a robust continuum based model should be able to predict the micro-damage healing process in addition to the damage evolution and growth. Here, we show that the micro-damage healing evolution law can easily be obtained from the principle of virtual power. In fact, the defined micro-damage healing microforce balance (Eq. (33)) is the balance law governing the micro-damage healing process in self-healing materials. The micro-damage healing microforce balance is recalled here as follows:

$$H - K = 0 \Rightarrow H^{\text{ene}} + (H^{\text{dis}} - K) = 0 \Rightarrow H^{\text{ene}} = -(H^{\text{dis}} - K) \quad (136)$$

where H^{ene} and H^{dis} are given in Eqs. (53) and (83), respectively. To the best of the authors' knowledge, this interesting result has been reported here for the first time. In fact, the micro-damage healing evolution function can be easily obtained using Eq. (136). Different forms for the micro-damage healing evolution function can be obtained based on the assumed mathematical forms for the thermo-healing Helmholtz free energy, Ψ^{th} , and the rate of thermo-healing energy dissipation, Π^{th} . In this paper, we assume the following mathematical forms for Ψ^{th} and Π^{th} in order to derive the micro-damage healing model proposed by Abu Al-Rub et al. (2010) to model fatigue damage in bituminous materials, such that:

$$\rho \Psi^{\text{th}} = \left[\frac{1}{k_1 + 1} \gamma_1 (1 - h)^{k_1 + 1} \right] \vartheta^{H,\text{ene}}; \quad \Pi^{\text{th}} = \left[\gamma_2 (1 - \phi)^{k_2} \dot{h}^2 \right] \vartheta^{H,\text{dis}} \quad (137)$$

where γ_1 , γ_2 , k_1 , and k_2 are material parameters. The parameters $\vartheta^{H,\text{ene}}$ and $\vartheta^{H,\text{dis}}$ are Arrhenius-type temperature coupling terms to couple temperature to the energetic and dissipative components of the micro-damage healing model. Note that the material parameters γ_1 and γ_2 could depend on the material's surface energy since they capture the changes in the total surface energy because of the healing of micro-cracks. Moreover, Π^{th} is expressed as a function of healing rate, \dot{h} , and damage history, $1 - \phi$. Energetic and dissipative components of the healing force can be obtained by substituting Eq. (137) into Eqs. (53) and (83), respectively, such that:

$$H^{\text{ene}} = -\gamma_1 (1 - h)^{k_1} \vartheta^{H,\text{ene}}; \quad H^{\text{dis}} - K = \gamma_2 (1 - \phi)^{k_2} \dot{h} \vartheta^{H,\text{dis}} \quad (138)$$

Substituting Eq. (138) into the micro-damage healing microforce balance (Eq. (136)) gives:

$$[\gamma_2 (1 - \phi)^{k_2} \vartheta^{H,\text{dis}}] \dot{h} - [\gamma_1 \vartheta^{H,\text{ene}}] (1 - h)^{k_1} = 0 \quad (139)$$

Eq. (139) defines the first-order differential equation governing the healing process. The healing evolution law can be obtained by rearranging Eq. (139) such that:

$$\dot{h} = \Gamma^h (1 - \phi)^{-k_2} (1 - h)^{k_1} \vartheta^H \quad (140)$$

where $\Gamma^h = \gamma_1 / \gamma_2$ is the micro-damage healing parameter and has the dimension 1/s and, hence, it controls the rate of micro-damage healing in materials, and $\vartheta^H = \vartheta^{H,\text{ene}} / \vartheta^{H,\text{dis}}$ is the healing temperature coupling term which can be defined as:

$$\vartheta^H = \exp \left[-\theta_4 \left(1 - \frac{T}{T_0} \right) \right] \quad (141)$$

The micro-damage healing evolution function is derived such that it considers the effect of short term healing as well as the long term time-dependent healing. In other words, Eq. (140) shows that at the beginning of the healing process the healing rate has its maximum value (i.e. $\dot{h} = \Gamma^h$). Therefore, the material instantaneously recovers part of its strength once put into rest. Eq. (140) shows that if the material is put into rest for a long time, the micro-damage healing continues with a decreasing rate as the healing variable increases. The history term (i.e. $(1 - h)^{k_1}$) is incorporated into the model to capture the time-dependent long term component of the micro-damage healing phenomenon.

This section concludes the derivation of the thermo-viscoelastic-viscoplastic-viscodamage-healing constitutive equations. It should be noted that this constitutive model is derived only as an example. However, the presented thermodynamic framework is general and can be used to derive different constitutive models.

5. Heat equation

As it was mentioned in previous sections, rate- and time-dependent materials show a wide range of mechanical responses depending on temperature. Changes in temperature could be caused by the changes in the ambient temperature or as a result of different forms of energy dissipation accompanied by the deformation process. Moreover, a local increase in temperature influences the behavior of materials during deformation. Hence, including the temperature evolution in the constitutive models seems inevitable for accurate modeling of time- and rate-dependent responses of such materials. In this section, the heat equation necessary for calculating the increase in temperature due to different deformation processes is derived.

We start from the first law of thermodynamic. The first law of thermodynamic for a sub-body Γ having the outward unit vector \mathbf{n} normal to the boundary $\partial\Gamma$ can be written as follows (Lemaître and Chaboche, 1990):

$$\frac{d}{dt} \int_{\Gamma} \rho e dV = P_{\text{ext}} - \int_{\partial\Gamma} q_i n_i dA + \int_{\Gamma} \rho r_{\text{ext}} dV \quad (142)$$

where e and r_{ext} are, respectively, the specific internal energy and the specific external heat gained by the body (e.g. through radiation), and P_{ext} is the external power presented in Eq. (19) which is equal to the internal power P_{int} in Eq. (20). Meanwhile, e , the specific entropy, η , and the Helmholtz free energy density, Ψ , are related through the following relationship (Lemaître and Chaboche, 1990):

$$\Psi = e - T\eta \quad (143)$$

Using the conservation of mass, using the divergence theorem, noting that the sub-body Γ is arbitrary, using the equivalency of internal and external expenditures of power, using the definition of internal expenditure of power in the healing configuration (Eq. (34)), and making use of damage and micro-damage healing balance laws (Eqs. (28) and (33)); the first law of thermodynamics, Eq. (142), can be rewritten as follows:

$$\rho(\dot{\Psi} + \dot{T}\eta + T\dot{\eta}) - \bar{\sigma}_{ij} \dot{\bar{\epsilon}}_{ij}^{ve} - \sum_{n=1}^{N_{\text{int}}^{ve}} \bar{\chi}_n \dot{\bar{\xi}}_n - \bar{X}_{ij} \dot{\bar{\epsilon}}_{ij}^{vp} - \bar{R} \dot{\bar{p}} - Y \dot{\phi} - (H - K) \dot{h} + q_{i,i} - \rho r_{\text{ext}} = 0 \quad (144)$$

Substituting Eqs. (46), (48), (64)–(68) into Eq. (144) yields:

$$\rho T \dot{\eta} = \Pi^{tve} + \Pi^{tvp} + \Pi^{tvd} + \Pi^{tH} + \rho r_{\text{ext}} - q_{i,i} \quad (145)$$

On the other hand, Eqs. (48) and (86) imply that the specific entropy can be decomposed into viscoelastic, viscoplastic, viscodamage, and micro-damage healing components, such that:

$$\eta = \eta^{tve} + \eta^{tvp} + \eta^{tvd} + \eta^{tH} \quad (146)$$

where η^{tve} , η^{tvp} , η^{tvd} , and η^{tH} are the specific entropies due to viscoelastic, viscoplastic, viscodamage, and micro-damage healing processes, respectively.

$$\eta^{tve} = -\frac{\partial \Psi^{tve}}{\partial T}; \quad \eta^{tvp} = -\frac{\partial \Psi^{tvp}}{\partial T}; \quad \eta^{tvd} = -\frac{\partial \Psi^{tvd}}{\partial T}; \quad \eta^{tH} = -\frac{\partial \Psi^{tH}}{\partial T} \quad (147)$$

The following equations for the specific entropy can be obtained by substituting Eqs. (87), (111), (128), and (137) into Eq. (147), such that:

$$\eta^{tve} = \frac{1}{\rho} \left[\frac{1}{2} a_0 (\bar{\epsilon}^{ve}) L_{ijkl}^{(1)} \bar{\epsilon}_{ij}^{ve} \bar{\epsilon}_{kl}^{ve} + \frac{1}{2} L_{mnn}^{(2)} \bar{\xi}_m \bar{\xi}_n + a_1 (\bar{\epsilon}^{ve}) L_{ijn}^{(3)} \bar{\epsilon}_{ij}^{ve} \bar{\xi}_n \right] Z^{ve} \quad (148)$$

$$\eta^{tvp} = \frac{1}{\rho} \left[\frac{1}{2} C_1 \bar{\epsilon}_{ij}^{vp} \bar{\epsilon}_{ij}^{vp} + \kappa_0 \bar{p} + \kappa_1 \left(\bar{p} + \frac{1}{\kappa_2} \exp(-\kappa_2 \bar{p}) \right) \right] Z^{vp} \quad (149)$$

$$\eta^{tvd} = \frac{1}{\rho b_1} (1 - \phi)^{b_1} \left[\frac{\bar{\tau}^{vd} - \alpha \bar{I}_1}{b_2} \right] \exp(b_3 \bar{\epsilon}_{\text{eff}}) Z^{vd} \quad (150)$$

$$\eta^{tH} = \frac{1}{\rho} \left[\frac{1}{k_1 + 1} \gamma_1 (1 - h)^{k_1 + 1} \right] Z^{H,\text{ene}} \quad (151)$$

where $Z = -\frac{\partial \Psi}{\partial T}$. Eqs. (148)–(151) reveal that:

$$\eta = \eta \left(\bar{\epsilon}_{ij}^{ve}, \bar{\epsilon}_{ij}^{vp}, \bar{p}, \phi, h, \bar{\xi}_n, T \right) \quad (152)$$

Taking the time derivative of Eq. (152) yields:

$$\dot{\eta} = \frac{\partial \eta}{\partial \bar{\epsilon}_{ij}^{ve}} \dot{\bar{\epsilon}}_{ij}^{ve} + \frac{\partial \eta}{\partial \bar{\epsilon}_{ij}^{vp}} \dot{\bar{\epsilon}}_{ij}^{vp} + \frac{\partial \eta}{\partial \bar{p}} \dot{\bar{p}} + \frac{\partial \eta}{\partial \phi} \dot{\phi} + \frac{\partial \eta}{\partial h} \dot{h} + \sum_{n=1}^{N_{\text{int}}^{ve}} \left(\frac{\partial \Psi}{\partial \bar{\xi}_n} \dot{\bar{\xi}}_n \right) + \frac{\partial \eta}{\partial T} \dot{T} \quad (153)$$

Substituting Eq. (153) into Eq. (145) and making use of Eqs. (50)–(53), and (147) gives the following thermo-mechanical heat balance equation:

$$\rho c_p \dot{T} = \Pi^{tve} + \Pi^{tvp} + \Pi^{tvd} + \Pi^{th} - \underbrace{\left[\frac{\partial \bar{\sigma}_{ij}^{ene}}{\partial T} \dot{\epsilon}_{ij}^{ve} + \frac{\partial \bar{\chi}_n}{\partial T} \dot{\zeta}_n + \frac{\partial \bar{X}_{ij}^{ene}}{\partial T} \dot{\epsilon}_{ij}^{vp} + \frac{\partial \bar{R}^{ene}}{\partial T} \dot{p} + \frac{\partial Y^{ene}}{\partial T} \dot{\phi} + \frac{\partial H^{ene}}{\partial T} \dot{h} \right]}_{\text{Thermo-mechanical coupling terms}} T + \rho r_{ext} - q_{i,i} \quad (154)$$

where $c_p = T \frac{\partial \eta}{\partial T}$ is the specific heat at constant pressure. Eq. (154) yields a physically sound relationship for the heat equation. This equation reveals two mechanisms that contribute to the changes in the rate of temperature: (a) the thermo-mechanical coupling terms which are functions of the energetic components of the thermodynamic conjugate forces; and (2) dissipation terms which are functions of the dissipative components of the thermodynamic conjugate forces appearing in different components of Π . The explicit relation for the heat equation can be easily obtained by substituting the energetic (Eqs. (89), (94)₁, (114)₁, (131), and (138)₁) and dissipative (Eqs. (94)₂, (98), (115), (133), and (138)₂) components of the thermodynamic conjugate forces into Eq. (154).

The relationship for the heat flux vector, \mathbf{q} , can be easily determined using the principle of maximum dissipation. Therefore, an expression is needed for the thermal component of the rate of energy dissipation in Eq. (84). We assume the following quadratic form for Π^{th} :

$$\Pi^{th} = \frac{1}{T} k_{ij}^{-1} q_i q_j \quad (155)$$

Substituting Eq. (155) into Eq. (84) yields:

$$q_i = -k_{ij} T_{,j} \quad (156)$$

where $\lambda^{th} = 1/2$. Eq. (156) is the well-known Fourier heat conduction law. The negative sign indicates that the heat flow is opposite to the direction of temperature increase.

6. Conclusion

In this work, we presented a general and comprehensive thermodynamic-based framework where special emphasis is placed on the decomposition of the thermodynamic conjugate forces into energetic and dissipative components to derive temperature-dependent viscoelastic, viscoplastic, viscodamage, and micro-damage healing constitutive equations for materials that also have the healing capability. This framework can be used to ensure the consistency of any proposed constitutive model within the laws of thermodynamics. Also, the proposed thermodynamic framework is completely based on only two main assumptions: (1) the knowledge of how the material stores energy, and thus a mathematical form can be postulated for the Helmholtz free energy function; and (2) the knowledge of how the material dissipates energy, and thus a mathematical form can be postulated for the rate of energy dissipation function.

We used the healing natural configuration proposed by Abu Al-Rub et al. (2010) as the extension of the well-known Kachanov’s effective (undamaged) configuration in order to enhance the continuum damage mechanics in modeling the micro-damage healing phenomenon. Hence, we presented the constitutive models in the healing configuration which substantially simplifies numerical implementation by avoiding the complexities associated with the direct couplings of viscoelastic and viscoplastic models to the viscodamage and micro-damage healing models. We used the power-correlating transformation hypothesis as proposed by Darabi et al. (2012) for relating the stress and strain tensors in the healing and damaged configurations. This hypothesis allowed us to present the constitutive model in the healing configuration (for simplicity) and yet to estimate positive definite dissipated energy in the healing natural configuration.

Moreover, we showed that the proposed thermodynamic formulation naturally enforces the decomposition of the thermodynamic conjugate forces into energetic and dissipative components. Energetic components are derived using the Helmholtz free energy. Furthermore, a systematic procedure based on the principle of maximum dissipation (or maximum entropy production) is presented for deriving dissipative components directly from the rate of energy dissipation. The thermodynamic framework is then used for deriving a more comprehensive version of Schapery-type viscoelastic model, Perzyna-type viscoplastic model, Darabi et al. (2011a) viscodamage model, and Abu Al-Rub et al. (2010) micro-damage healing model. Moreover, all the derived constitutive models are coupled to temperature. It is shown that the presented thermodynamic framework yields a simpler form for temperature-dependent viscoelastic models where there is no need for using the temperature-shift factor in the definition of the so-called reduced time in thermo-viscoelastic models. Instead, an Arrhenius-type (or any form) temperature coupling term can be used for making the viscoelasticity model as temperature-dependent.

Furthermore, for the first time, it is shown that the principle of virtual power can be used for deriving generalized non-associative viscoplasticity theories without further assuming a viscoplastic potential function independent from the yield loading condition. We also showed that the rate-dependent terms in viscoplasticity dynamic yield surface are identical to the dissipative components of the hardening function and can be derived directly from the rate of energy dissipation. Moreover, an equation for the evolution of the backstress is proposed which can be considered as a more general version of Armstrong and Frederick (1966) model for kinematic hardening.

We derived the viscoelastic model using the viscoelastic microforce balance, obtained directly from the principle of virtual power. Similarly, we derived the viscodamage and micro-damage healing loading conditions and evolution laws using the viscodamage microforce balance and micro-damage healing microforce balance, respectively. To the author's best knowledge, the microforce balances for viscoelasticity and micro-damage healing are new and have not been presented before.

Moreover, the well-known Fourier heat conduction law is derived as a consequence of decomposing thermodynamic conjugate forces into energetic and dissipative components and using the principle of maximum dissipation. Finally, a general form for the heat equation is derived.

The derived constitutive equations in Section 4 are extensively validated in the second part of this paper.

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Appendix A. Non-associative plasticity/viscoplasticity based on the principle of virtual power

One of the challenges in the associative plasticity/viscoplasticity theories is that these theories cannot accurately predict the plastic strain in pressure-dependent materials such as polymers, soils, rocks, bituminous materials, and geomaterials (e.g. Zienkiewicz et al., 1975; Oda and Nakayama, 1989; Cristescu, 1994; Florea, 1994; Pestana and Whittle, 1999; Collins and Kelly, 2002; Dormieux et al., 2006). To overcome this issue, a plastic potential function different from the yield function is usually assumed to obtain the accurate amount of plastic strain using a non-associative flow rule. This plastic potential function is selected, so far, solely based on experiments. However, as it was mentioned earlier, the basic assumption in Ziegler's thermodynamic approach (Ziegler, 1983) for deriving constitutive models for materials is that they are fully determined by the knowledge of a thermodynamic potential such as the Helmholtz free energy function and another function which is the dissipation function. For associative plasticity theories, however, this assumption yields the normality rule which can be considered as the direct consequence of the thermodynamic orthogonality principle (Ziegler, 1981) which states that the plastic strain tensor is always normal to the yield surface. Obviously, the normality of the plastic strain to the yield surface does not hold for pressure-sensitive materials such as geomaterials. Several researchers have derived associative plasticity/viscoplasticity flow rules based on the principle of virtual power (e.g. Gurtin, 2000, 2002; Gurtin and Anand, 2005; Voyiadjis and Abu Al-Rub, 2007). We will show here that the generalized non-associative plastic/viscoplastic theories can be a direct consequence of the principle of virtual power.

The associative plasticity theories assume that the direction of the plastic strain \mathbf{N} is normal to the yield surface. Let us assume for simplicity and without loss of generality that the material is simply elasto-plastic with isotropic hardening only. Hence, for this material, the principle of virtual power can be written as follows:

$$\int_{\Gamma} (\sigma_{ij} \delta \dot{\epsilon}_{ij}^e + R \delta \dot{p}) dV = \int_{\Gamma} b_i \delta \dot{u}_i dV + \int_{\partial \Gamma} t_i \delta \dot{u}_i dA - \int_{\Gamma} \rho \ddot{u}_i \delta \dot{u}_i dV \quad (\text{A.1})$$

where $\dot{\epsilon}^e$ is the elastic strain tensor. Using the additive strain decomposition into elastic, ϵ^e , and plastic, ϵ^p , components, substituting the macroforce balance (Eq. (25)) and the macroscopic boundary traction equation (Eq. (26)) into Eq. (A.1) yields:

$$\sigma_{ij}^* \delta \dot{\epsilon}_{ij}^p = 0 \quad (\text{A.2})$$

where σ^* is given by

$$\sigma_{ij}^* = \sigma_{ij} - \sqrt{\frac{2}{3}} R N_{ij} \quad (\text{A.3})$$

Eq. (A.2) should be satisfied for all possible cases. Three possible cases which may always make this equation zero are investigated in the following:

(a) Case 1:

$$\delta \dot{\epsilon}_{ij}^p = 0_{ij} \quad (\text{A.4})$$

However, the field $\delta \dot{\epsilon}^p$ can be selected arbitrary. Therefore, this case cannot always be satisfied.

(b) Case 2:

$$\sigma_{ij}^* = 0_{ij} \quad (\text{A.5})$$

This case gives a plastic flow rule (or a microforce balance), different than the flow rule in Eq. (27), and enforces the co-directionality constraint by requiring that the direction of the plastic strain \mathbf{N} coincides with the direction of the stress tensor $\boldsymbol{\sigma}$. Therefore, from Eqs. (A.3) and (A.5), we can write for this case:

$$N_{ij} = \sqrt{\frac{3}{2}} \frac{\sigma_{ij}}{R} \tag{A.6}$$

Moreover, for this case, one can define the yield function f by taking the Euclidean norm of Eq. (A.5) along with Eq. (A.3) and noting that $\|\mathbf{N}\| = 1$, such that:

$$f = \sqrt{\frac{3}{2}} \|\sigma_{ij}\| - R = 0 \tag{A.7}$$

However, this expression shows that Case 2, Eq. (A.5), yields an associative plastic flow rule and the normality condition, where one can obtain from Eq. (A.7) that the direction of the plastic flow is normal to the yield surface f , such that:

$$\hat{N}_{ij} = \frac{\partial f}{\partial \sigma_{ij}} = \frac{\sigma_{ij}}{\|\sigma_{ij}\|} = \sqrt{\frac{3}{2}} \frac{\sigma_{ij}}{R} = N_{ij} \tag{A.8}$$

Eq. (A.6) is also used in obtaining the above restriction.

(c) Case 3:

Another possible case, which is also the most general, is that the stress tensor $\boldsymbol{\sigma}^*$ be perpendicular to the rate of the plastic strain or equivalently to the direction of the plastic strain rate (i.e. $\boldsymbol{\sigma}^* \perp \mathbf{N}$). This does not necessarily imply that the plastic flow direction coincides with the direction of the stress tensor $\boldsymbol{\sigma}$. Eq. (A.2) can be rewritten as the inner product of \mathbf{N} and $\boldsymbol{\sigma}^*$ by utilizing Eq. (23), such that:

$$\sigma_{ij}^* N_{ij} = 0 \tag{A.9}$$

However, the microforce balance in Eq. (27), which is equivalent to the yield function f , can be obtained from Eq. (A.9) and noting that $\mathbf{N}:\mathbf{N} = 1$, such that:

$$f = \sigma_{ij}^* N_{ij} = \hat{\sigma} - \sqrt{\frac{2}{3}} R = 0 \tag{A.10}$$

where $\hat{\sigma}$ is termed as the resolved or equivalent stress since it represents the stress $\boldsymbol{\sigma}$ resolved in the direction of the plastic flow \mathbf{N} , and is given by:

$$\hat{\sigma} = \sigma_{ij} N_{ij} \tag{A.11}$$

It is obvious from Eq. (A.10) that the normal to the yield surface (i.e. $\hat{\mathbf{N}} = \partial f / \partial \boldsymbol{\sigma}$) does not coincide with the direction of the plastic strain rate (or equivalently is not the same as \mathbf{N}). In case \mathbf{N} is co-directional with $\boldsymbol{\sigma}$, then from Eq. (A.11) we obtain $\hat{\sigma} = \|\boldsymbol{\sigma}\|$, which is the case in Eq. (A.7). We can also relate $\hat{\mathbf{N}}$ and \mathbf{N} from Eq. (A.10) as follows:

$$\hat{N}_{ij} = N_{ij} + \sigma_{kl} \frac{\partial N_{kl}}{\partial \sigma_{ij}} \tag{A.12}$$

This general case is schematically presented in Fig. 4 in the σ_{ij} space.

The yield function f in Eq. (A.7) or Eq. (A.10) is, therefore, equivalent to the plastic potential F only for the case of associative plasticity (i.e. $\mathbf{N} = \hat{\mathbf{N}}$). In other words, taking the Euclidean norm of Eq. (A.10) yields:

$$\|\sigma_{ij}\| \geq \sqrt{\frac{2}{3}} R \tag{A.13}$$

which implies that $\|\boldsymbol{\sigma}\|$ is not the equivalent stress as it is in the case of Eq. (A.7). Also, this inequality reduces to an equality when $\boldsymbol{\sigma}$ is co-directional with \mathbf{N} . However, for the general case, Eq. (A.13) remains an inequality.

Now, let F be a plastic potential function, such that we can define:

$$N_{ij} = \frac{\partial F}{\partial \sigma_{ij}} \tag{A.14}$$

Then the plastic strain rate is given from Eq. (23) as follows:

$$\dot{\epsilon}_{ij}^p = \sqrt{\frac{3}{2}} \dot{p} \frac{\partial F}{\partial \sigma_{ij}} \tag{A.15}$$

The constraint between the plastic potential function F and the yield surface function f can be obtained by substituting Eq. (A.14) into Eq. (A.9) along with Eq. (A.3), such that:

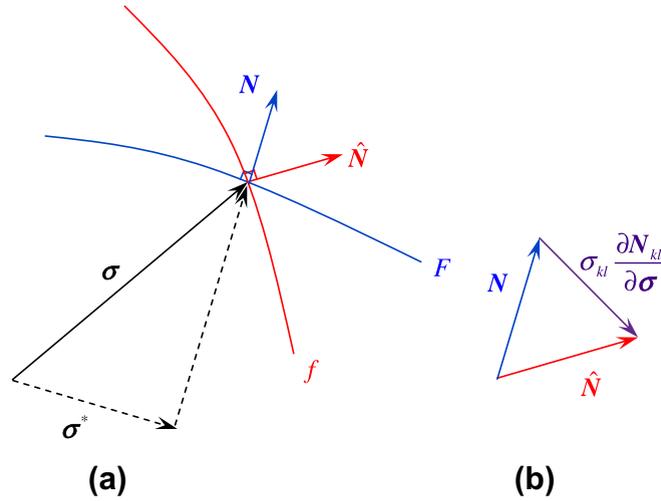


Fig. 4. (a) Schematic representation of the relationship between different components of the stress tensor with unit tensors normal to the yield surface f and plastic potential F functions in the σ_{ij} space and (b) relationship between the unit tensors normal to the yield, N , surface and plastic potential, \hat{N} , in the σ_{ij} space for the generalized nonassociative plasticity theories.

$$f = \sigma_{ij} \frac{\partial F}{\partial \sigma_{ij}} - \sqrt{\frac{2}{3}} R = 0 \quad (\text{A.16})$$

Differentiating both sides of Eq. (A.16) with respect to σ or, equivalently, substituting Eq. (A.14) into Eq. (A.12) yields:

$$\frac{\partial f}{\partial \sigma_{ij}} = \frac{\partial F}{\partial \sigma_{ij}} + \sigma_{kl} \frac{\partial^2 F}{\partial \sigma_{kl} \partial \sigma_{ij}} \quad (\text{A.17})$$

Eq. (A.17) provides the constraint between the yield function f and the plastic potential function F for non-associative/associative plasticity/viscoplasticity theories.

As it was discussed earlier, in the associative plasticity theories, the yield function f and the plastic potential function F are assumed to be the same or, equivalently, the direction of plastic flow is normal to the yield surface (i.e. $N = \partial F / \partial \sigma = \partial f / \partial \sigma$). According to Eq. (A.17), the assumption of associative plasticity requires that the second term in the right-hand-side of Eq. (A.17) be zero, such that:

$$\sigma_{kl} \frac{\partial^2 F}{\partial \sigma_{kl} \partial \sigma_{ij}} = 0_{ij} \text{ when } f = F \quad (\text{A.18})$$

or equivalently from Eq. (A.12):

$$\sigma_{kl} \frac{\partial N_{kl}}{\partial \sigma_{ij}} = 0 \text{ when } \hat{N}_{ij} = \frac{\partial f}{\partial \sigma_{ij}} = \frac{\partial F}{\partial \sigma_{ij}} = N_{ij} \quad (\text{A.19})$$

which implies that $\sigma \perp \frac{\partial N}{\partial \sigma}$ as the basic assumption for associative plasticity theories. Hence, we can conclude that Eq. (A.17) governs the relation between the yield surface f and plastic potential function F in both associative and non-associative plasticity. It should be mentioned that this equation naturally implies that the yield surface and the plastic potential functions are the same for associative plasticity.

The above arguments clearly show the existence of a constraint between the yield function f and the plastic potential function F in a thermodynamically consistent framework. The yield surface f can be derived directly using the microforce balance in Eq. (27) without the need for any further assumption other than the Helmholtz free energy function and the rate of the energy dissipation that will be shown in the subsequent development. On the other hand, one may solve the differential equation presented in Eq. (A.17) for thermodynamically admissible potential functions F once the yield function is known. Reversely, one can use the given plastic potential function to derive its associated thermodynamically admissible yield function f . The second approach is used in this paper to derive the thermodynamically consistent yield functions associated with the given plastic potential function.

It is worth noting that the traditional approach is to select the yield surface directly based on the experimental measurements. Subsequently, a plastic potential is usually assumed using non-associative plasticity, which is very often chosen similar to the yield surface, to match the experimental data. While it can be argued that the traditional approach might be easier, there is no guarantee for the selected yield surface and plastic potential functions to satisfy the thermodynamic laws. The approach presented in this paper can be used in conjunction with the traditional approach. In other words, once the yield

surface function is determined based on the experimental measurements, the associated thermodynamically consistent plastic potential can be derived based on the presented approach. The derived plastic potential function can then be validated against the experimental data. This approach provides a useful tool to derive thermodynamically consistent plastic potentials instead of simply assuming one. Also, even if the experimental measurements do not compare well with the prediction of the derived plastic potential, the derived function can be regarded as a guideline to assume a form for the plastic potential with the confidence that the assumed plastic potential does not violate the thermodynamic laws and can be used for more general loading scenarios.

It should be noted that the same arguments can be made for deriving associative and non-associative damage rules for the case of anisotropic damage (Voyiadjis et al., 2004).

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