Chapter 3 State Variables Approach

The State Variables approach is an alternative to the history dependent integral representation given in Chap. 2. It has a physical basis because of its origin in thermodynamic formulations and shows computational advantages. The creep and relaxation functions are approximated by exponential series. The introduction of state variables leads to *n* differential equations of first order in place of the differential equation of order *n* linked to a generalized model. This formulation leads to exponential expressions that make incremental integration easier, allowing the determination of the viscoelastic strains at time $t + \Delta t$ as a function of the viscoelastic strains and stresses at time *t*. Then, there is no need to store the whole history of stress or strain. In this chapter, we introduce the basic formulation that is later extended to 3D, aging and nonlinear situations.

3.1 Basic Formulation

We have already seen (Chap. 2) that for each rheological model, we may have an integral as well as a differential relation. We shall see now how to obtain, through the State Variables approach, a new general form convenient for computational applications.

In some important commercial computer codes (i.e. Abaqus, Ansys) the theoretical formulation is introduced in the integral form. Then, reference is made to a rheological model (generalized Maxwell) and Prony series are introduced as its representation. The State Variables approach [1, 3] presented here helps us to understand better the relation among these formulations.

Let us begin with the general form of the integral representation (see (2.6))

$$\varepsilon(t) = \frac{\sigma(t)}{E_0} + \int_{\tau_0}^t d(t-\tau)\sigma(\tau)d\tau$$
(3.1)

where $E_0 = E(\tau_0)$.

We may approximate the function $d(t - \tau)$ by means of an exponential series (called Dirichlet-Prony series by mathematicians)

$$d(t - \tau) = \sum_{i=1}^{n} d_i e^{\frac{(t - \tau)}{\theta_i}}$$
(3.2)

Such an approximation is *complete* (i.e. can be as good as we like, depending on the number of terms included). We introduce then the n values

$$q_i(t) = \int_{\tau_0}^t d_i e^{-\frac{(t-\tau)}{\theta_i}} \sigma(\tau) d\tau \quad i = 1, \dots, n$$
(3.3)

and notice that, by taking the differential of (3.3) with relation to *t* (using Leibnitz rule, Appendix A) we obtain

$$\dot{q}_i(t) + \frac{q_i(t)}{\theta_i} = d_i \sigma(t) \quad i = 1, \dots, n$$
(3.4)

which is a system of *n* uncoupled linear differential equations of the first degree that, with the adequate initial conditions (e.g. $q_i = 0$ for $t = \tau_0$) allows us to determine the state variables. Then, with

$$\varepsilon(t) = \frac{\sigma(t)}{E_0} + \sum_{i=1}^n q_i(t)$$
(3.5)

that results from (3.1), (3.2) and (3.3) the strain can be determined.

Moreover, we notice that:

- (i) Equations (3.4) and (3.5) correspond in this case to a generalized Kelvin Model with springs of constants $1/d_i\theta_i$ and dashpots with constants $1/d_i$ and an isolated spring of constant E_0 .
- (ii) From (3.4) and (3.5) we see also that, when the values q_i are known at a given instant t_r , then $\varepsilon(t)$ may be determined for $t \ge t_r$ if $\sigma(t)$ is known for $t \ge t_r$. Thus, if the strains are measured for $t \ge t_r$ with respect to the configuration at t_r , the material behavior in the interval (t_r, t_f) with $t_f > t_r$ will depend only on the value of the stresses in (t_r, t_f) and the value of q_i at time t_r . The observations above justify the name *state variables* representation.
- (iii) This representation is very general and can be extended to aging and nonlinear problems as well (see Chaps. 7 and 8).
- (iv) State variables may also be related to the material microstructure [5].

3.1 Basic Formulation

(v) Finally, this formulation is convenient for the numerical solution of viscoelastic problems (using for example the Finite Element Method).

Alternatively, we may begin with the relation

$$\sigma(t) = \int_{\tau_0}^t E(t-\tau)\dot{\varepsilon}(\tau)d\tau$$
(3.6)

and expand

$$E(t) = E_{\infty} + \sum_{i=1}^{n} E_i e^{-t/T_i}$$
(3.7)

Introducing the *n* quantities

$$q_i(t) = \int_{\tau_0}^t e^{-\frac{(t-\tau)}{T_i}} \dot{\varepsilon}(\tau) d\tau \quad i = 1, \dots, n$$
(3.8)

and taking the derivative of (3.8) with respect to t we obtain

$$\dot{q}_i(t) + \frac{q_i(t)}{T_i} = \dot{\varepsilon}(t) \quad i = 1, \dots, n$$
 (3.9)

A combination of (3.6), (3.7) and (3.8) provides the equation

$$\sigma(t) = E_{\infty}\varepsilon(t) + \sum_{i=1}^{n} E_{i}q_{i}(t)$$
(3.10)

Equations (3.9) and (3.10) together with the initial conditions $q_i = 0$ when $t = \tau_0$ correspond to a Maxwell generalized model with springs E_i , dashpots T_iE_i and an isolated spring E_{∞} . Here q_i represents the strains in the springs of the Maxwell elements.

3.2 Incremental Determination of State Variables

We may integrate system (3.4) in a variety of ways.

1. The use of the simple Euler process gives us, for a step increment $\Delta t,$ the algorithm

$$\Delta q_i(t) = -\left(\frac{q_i(t)}{\theta_i} - d_i\sigma(t)\right)\Delta t$$

$$q_i(t + \Delta t) = q_i(t) + \Delta q_i(t)$$
(3.11)

2. Better results are obtained writing

$$q_i(t+\Delta t) = \int_{\tau_0}^t d_i e^{-(t+\Delta t-\tau)/\theta_i} \sigma(\tau) d\tau + \int_t^{t+\Delta t} d_i e^{-(t+\Delta t-\tau)/\theta_i} \sigma(\tau) d\tau$$
(3.12)

The first integral is equal to $q_i \exp(-\Delta t/\theta_i)$; the second one may be written, assuming $\sigma(t)$ constant over the interval $[t, t + \Delta t]$, as

$$d_i \sigma(t) e^{-(t+\Delta t)/\theta_i} \int_{t}^{t+\Delta t} e^{\tau/\theta_i} d\tau = d_i \theta_i \sigma(t) (1 - e^{-\Delta t/\theta_i})$$
(3.13)

so that

$$q_i(t + \Delta t) = e^{-\Delta t/\theta_i} q_i(t) + d_i \theta_i \sigma(t) (1 - e^{-\Delta t/\theta_i})$$
(3.14)

Expressions of this type are used in some viscoelastic computer codes (e.g. Ansys). Simo and Hughes [6] propose an alternative of the same accuracy. The value of a state variable at a given time may be determined directly from its value at the previous time step and the history of stress or strain; this incremental procedure is more accurate than the Euler integration procedure and is more efficient than the direct numerical calculation of the integral in (3.3).

3. A more efficient algorithm may be obtained considering the relation $\sigma(\tau)$ to vary linearly in the interval $[t, t + \Delta t]$

$$\sigma(\tau) = \sigma(t) + \overline{\Delta\sigma}(t)(\tau - t); \quad t \le \tau \le t + \Delta t$$
(3.15)

where

$$\overline{\Delta\sigma}(t) = \left[\sigma(t) - \sigma(t - \overline{\Delta t})\right] / \overline{\Delta t}$$
(3.16)

and $\overline{\Delta t}$ is the time interval in the preceding step. Then, (3.16) takes the form

$$q_{i}(t + \Delta t) = e^{-\Delta t/\theta_{i}}q_{i}(t) + \sigma(t)d_{i}\theta_{i}\left(1 - e^{-\Delta t/\theta_{i}}\right) + \frac{\left[\sigma(t) - \sigma(t - \overline{\Delta t})\right]d_{i}\theta_{i}}{\overline{\Delta t}}\left[\Delta t - \theta_{i}\left(1 - e^{-\Delta t/\theta_{i}}\right)\right]$$
(3.17)

The determination of the value of the state variable $q(t + \Delta t)$ in an incremental process requires the knowledge of $q(t), \overline{\Delta t}, \sigma(t)$ and $\sigma(t - \overline{\Delta t})$. A similar algorithm is used in Abaqus. Other algorithms may be found in [7].

3.3 Physical Grounds and Extensions

Many inelastic properties of solids can be explained qualitatively in terms of various micro-structural rearrangements. In polymers, for example, the existence of long-chain molecules, which may straighten or crumple, in addition to sliding relatively to each other in response to sustained loads, provides the material with instantaneous elasticity as well as with nonlinear viscosity. During these processes, a certain amount of mechanical energy is lost into thermal energy. Additionally, the micro-structural changes give rise to macroscopic history-dependent material properties [2].

Explicit representations of history dependence may be formulated on purely mathematical assumptions and expressed as integrals of stress or strain history, as shown in Chap. 2, 7 and 8. Alternatively, a state variables representation may be used with some advantages in viscoelasticity as well as in plasticity and damage mechanics.

Then, the effect of the microscopic structural rearrangements is accounted for by the introduction of additional *n* state variables called internal variables or hidden coordinates, denoted collectively by $q_i(i = 1, ..., n)$ which, in a certain average global sense, represent the internal changes. The optimal selection of suitable internal variables, minimum in number, which provide maximum information, is an important problem [4].

Once the internal variables are chosen, we may define stress and internal energy as

$$\sigma = \sigma(\varepsilon, \Theta, q_i)$$

$$\Psi = \Psi(\varepsilon, \Theta, q_i)$$
(3.18)

where stress and free energy are expressed as functions of current values of strain (stress), temperature and other variables, including the internal state variables.

Rate effects are introduced through *evolution* or *growth laws*, in terms of the history of external quantities like the stress or strain tensors and temperature, as follows:

$$\dot{q}_i(t) = f(q_i, \Theta, \varepsilon) \tag{3.19}$$

From this set of equations one may explicitly eliminate the internal variables from the constitutive equations, thus obtaining a result similar to that from the functional theory in which stress (strain) is expressed as a functional of strain (stress).

An advantage of the state variable approach is that physical theories, and microstructural information, may be introduced directly in the formulation of the evolution equations. Another one is that it leads to more efficient numerical procedures. This formulation will be extended to nonlinear viscoelasticity in Chap. 8. In the finite strain situations it is important to take account of rigid rotations and the related concepts of *State and Orientation* [5].

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