Creep User Subroutine Model for Shrinkage Microporosity

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Terms and Symbols

AM	m	exponent for the plasticity term
AN	n	exponent for the creep term
DECRA(1)	$\Delta\varepsilon^{cr}$	effective creep strain increment
DECRA(4)	$\left(\dfrac{\partial\Delta\varepsilon^{cr}}{\partial(-\sigma_m)}\right)_{\sigma_e}$	partial derivative of $\Delta\varepsilon^{cr}$ with respect to σ_m
DECRA(5)	$\left(\dfrac{\partial\Delta\varepsilon^{cr}}{\partial\sigma_e}\right)_{-\sigma_m}$	partial derivative of $\Delta\varepsilon^{cr}$ with respect to σ_e
DESWA(1)	$\Delta\varepsilon^{sw}$	volumetric (or swelling) strain increment
DESWA(4)	$\left(\dfrac{\partial\Delta\varepsilon^{sw}}{\partial(-\sigma_m)}\right)_{\sigma_e}$	partial derivative of $\Delta\varepsilon^{sw}$ with respect to σ_m
DESWA(5)	$\left(\dfrac{\partial\Delta\varepsilon^{sw}}{\partial(\sigma_e)}\right)_{-\sigma_m}$	partial derivative of $\Delta\varepsilon^{sw}$ with respect to σ_e
ED0	$\dot\varepsilon_0$	effective characteristic reference strain rate for the creep term
ED0L	$\dot\varepsilon_{0l}$	characteristic reference strain rate for complete liquid material
ED0S	$\dot\varepsilon_{0s}$	characteristic reference strain rate for complete solid material
EDP	$\dot\varepsilon_p$	effective characteristic reference strain rate for the plasticity term
ENERGY	Q	activation energy
G2	$g_2(\rho)$	
G2P	$g_{2p}(\rho)$	
G3	$g_3(\rho)$	
G3P	$g_{3p}(\rho)$	
GASCON	R	universal gas constant
P	$-\sigma_m$	pressure
QTILD	σ_e	Mises stress
RHO	ρ	effective porosity
RHOP	ρ_p	porous free space fraction of total material
RHOL	ρ_l	liquid fraction of total material
SIG0	σ_0	characteristic reference stress for the creep term
SIGB	$\bar\sigma$	
SIGBP	$\bar\sigma_p$	
SIGP	σ_P	characteristic reference stress for the plasticity term
T	(N/A)	mid-of-increment temperature
TEMP	T	material temperature
TEMP0	T_0	reference temperature at σ_0
TEMP1	T_1	first liquid pore formation temperature
TEMP2	T_2	last liquid pore formation temperature
TEMPM	T_m	melting temperature
TEMPS	T_s	solidus temperature
TEMPX	(N/A)	temperature at the end of an increment

Introduction

The model is organised in a way to utilise the Abaqus CREEP USER subroutine (or UMAT) as a platform which provides an implicit time integration scheme of creep and swelling behaviour. In this subroutine nonlinear equations will be solved at each time increment, and the variations of the effective creep strain increment $\Delta\varepsilon^{cr}$ ($= \dot{\varepsilon}_e dt$) and volumetric (or swelling) strain increment $\Delta\varepsilon^{sw}$ ($= \dot{\varepsilon}_v dt$) with respect to the von Mises effective stress σ_e and the mean (or hydrostatic component of) stress σ_m must be defined. This requires specifying the effective strain rate $\dot{\varepsilon}_e$ and the volumetric strain rate $\dot{\varepsilon}_v$ as a function of σ_e, σ_m, temperature T and any state variables. The routine must also provide the evolution law for the state variables.

If the material is fully dense the constitutive response can be expressed as the following, in two terms: at high temperature where the material goes through creep deformation,

$$\dot{\varepsilon}_{e,high} = A\sigma_e{}^n = \dot{\varepsilon}_0 \left(\frac{\sigma_e}{\sigma_0}\right)^n exp\left[-\frac{Q}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \qquad \text{[1]A}$$

at low temperature in which case the material experiences perfect plastic deformation,

$$\dot{\varepsilon}_{e,low} = B\sigma_e{}^m = \dot{\varepsilon}_p \left(\frac{\sigma_e}{\sigma_p}\right)^m \qquad \text{[1]b}$$

where $\dot{\varepsilon}_e = \sqrt{\frac{2}{3}\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}}$ is the effective strain rate, $\sigma_e = \sqrt{\frac{3}{2}s_{ij}s_{ij}}$ is the effective stress with $s_{ij} = \sigma_{ij} - \sigma_m\delta_{ij}$ representing the deviatoric stress tensor, $\sigma_m = \frac{1}{3}\sigma_{kk}$ is the mean stress and δ_{ij} is the Kroneker delta. $\dot{\varepsilon}_0$ is the effective strain rate at a stress σ_0 and temperature T_0, n is the creep exponent typically in the range 3 to 18, Q is the activation energy for creep and R is the universal gas constant. $\dot{\varepsilon}_p$ is the strain rate at σ_p, m is the plasticity exponent typically in the range 100 to 600. Since σ_e is much lower at high temperature than at low temperature, σ_0 is significantly lower than σ_p. The following diagram shows an approximate relationship between $\dot{\varepsilon}_e$ and σ_e.
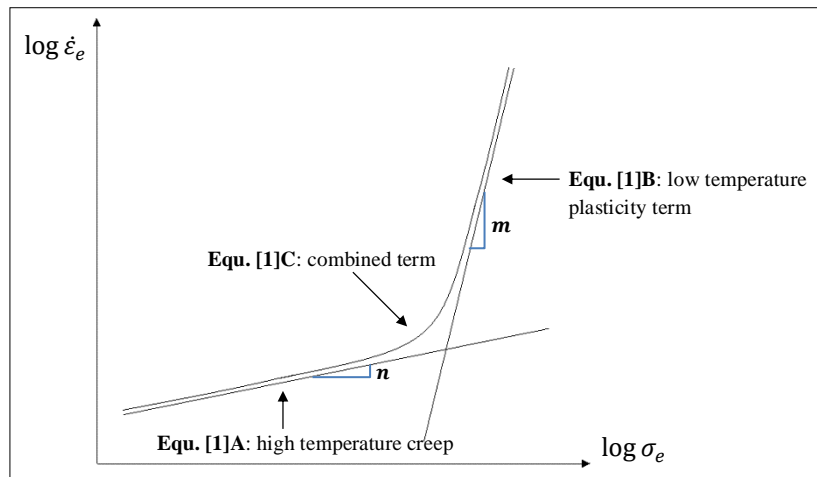

Figure 1 Constitutive response of the materials incorporating two types of deformation

As shown in **Figure 1**, combining the two terms would give the total constitutive response for a fully dense material, as shown below:

$$\dot{\varepsilon}_e = A\sigma_e{}^n + B\sigma_e{}^m = \dot{\varepsilon}_0 \left(\frac{\sigma_e}{\sigma_0}\right)^n exp\left[-\frac{Q}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] + \dot{\varepsilon}_p \left(\frac{\sigma_e}{\sigma_p}\right)^m \qquad \text{[1]c}$$

Physics of the Model

Consider the situation where the material is cooled from the melt. Initially, if the material is deformed liquid can flow between the dendrites to completely fill space and accommodate any local volume change. As it is cooled and the dendrites grow, pockets of liquid become fully enclosed by solid. Liquid is then unable to flow in order to accommodate any volume change. Assume that the liquid is unable to support any tensile stresses. Also ignore, at this stage, any volume change as the material solidifies. The solid skeleton then behaves as a porous creeping material. The porosity can grow under an applied stress (provided there is a positive mean stress) and it can reduce as the result of additional material solidifying within the pores.

At a given instant the material behaves as a porous material. Let ρ be the porosity (ratio of pore volume to total volume). The constitutive response can then be expressed in the form

$$\dot{\varepsilon}_e = \dot{\varepsilon}_0 \left(\frac{\bar{\sigma}}{\sigma_0}\right)^{n-1} \frac{\sigma_e}{\sigma_0 g_2(\rho)} exp\left[-\frac{Q}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] + \dot{\varepsilon}_p \left(\frac{\bar{\sigma}_p}{\sigma_p}\right)^{m-1} \frac{\sigma_e}{\sigma_p g_{2p}(\rho)} \qquad [2]A$$

$$\dot{\varepsilon}_v = \dot{\varepsilon}_0 \left(\frac{\bar{\sigma}}{\sigma_0}\right)^{n-1} \frac{\sigma_m}{\sigma_0 g_3(\rho)} exp\left[-\frac{Q}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] + \dot{\varepsilon}_p \left(\frac{\bar{\sigma}_p}{\sigma_p}\right)^{m-1} \frac{\sigma_e}{\sigma_p g_{3p}(\rho)} \qquad [2]b$$

where $\bar{\sigma} = \sqrt{\frac{\sigma_e^2}{g_2(\rho)} + \frac{\sigma_m^2}{g_3(\rho)}}$, $g_2(\rho) = \frac{(1-\rho)^{\frac{2n}{n+1}}}{\left(1+\frac{2}{3}\rho\right)}$, $g_3(\rho) = \frac{4}{9}\left[n\left(\rho^{-\frac{1}{n}} - 1\right)\right]^{\frac{2n}{n+1}}$; $\bar{\sigma}_p = \sqrt{\frac{\sigma_e^2}{g_{2p}(\rho)} + \frac{\sigma_m^2}{g_3(\rho)}}$, $g_{2p}(\rho) =$

$\frac{(1-\rho)^{\frac{2m}{m+1}}}{\left(1+\frac{2}{3}\rho\right)}$, $g_{3p}(\rho) = \frac{4}{9}\left[m\left(\rho^{-\frac{1}{m}} - 1\right)\right]^{\frac{2m}{m+1}}$ (see references above for their origins).
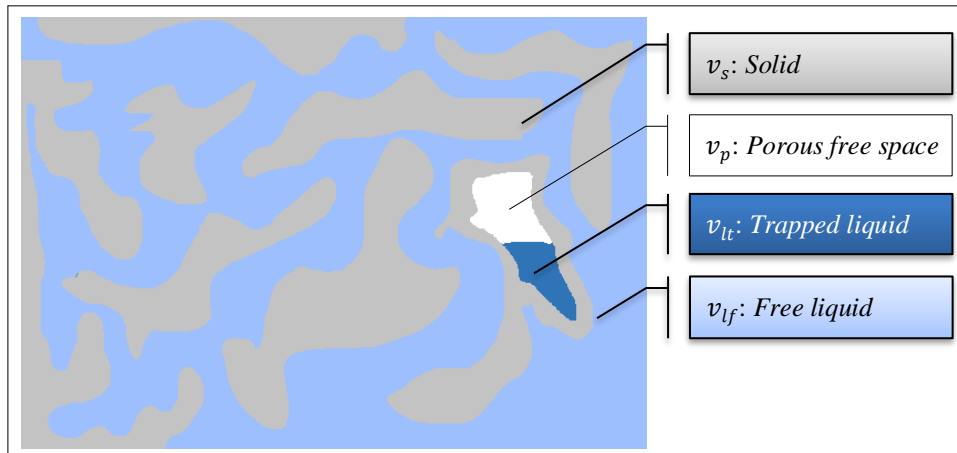

Figure 2 Materials illustration at temperature T_1 as the first liquid pore forms

Assume that the first liquid pocket forms at a temperature T_1, and that as the material is cooled below this temperature, the last liquid pocket forms at a temperature T_2, whilst complete solidification occurs at the solidus temperature T_s.

At temperature below T_1 the material is partially porous and its effective porosity ρ changes as a result of both the deformation and as a result of the solidification of liquid within the pores:

$$\rho = \rho_p + \rho_l = \frac{v_p + v_{lt}}{V} = \frac{v_p + v_{lt}}{v_p + v_l + v_s} \qquad [3]$$

$$\text{Note: } v_l = v_{lt} + v_{lf} \qquad [4]$$

where v_p is the volume occupied by porous free space, v_l is the volume of liquid of which v_{lt} is the volume of liquid trapped inside the pores, v_{lf} is the volume of liquid flowing freely between dendrite channels, and v_s is the volume of solid. V is the total volume of the material. As seen in **Figure 2**.

Differentiating ρ_p and noting that $\dot{v}_s = -\dot{v}_l$ gives

$$\dot{\rho}_p = \frac{\dot{v}_p}{V}\left(1 - \frac{v_p}{V}\right)$$ [5]

as $\dot{\varepsilon}_v = \frac{\dot{v}_p}{V}$, equation [5] can be written in terms of the variables that the USER subroutine deals with:

$$\dot{\rho}_p = \dot{\varepsilon}_v(1 - \rho_p)$$ [6]

Note that there is no need to differentiate ρ_l, instead, if the general relationship between the volume fraction of liquid and temperature is assumed as linear, a transition of the volume fraction of liquid with respect to temperature can be assumed as follows:
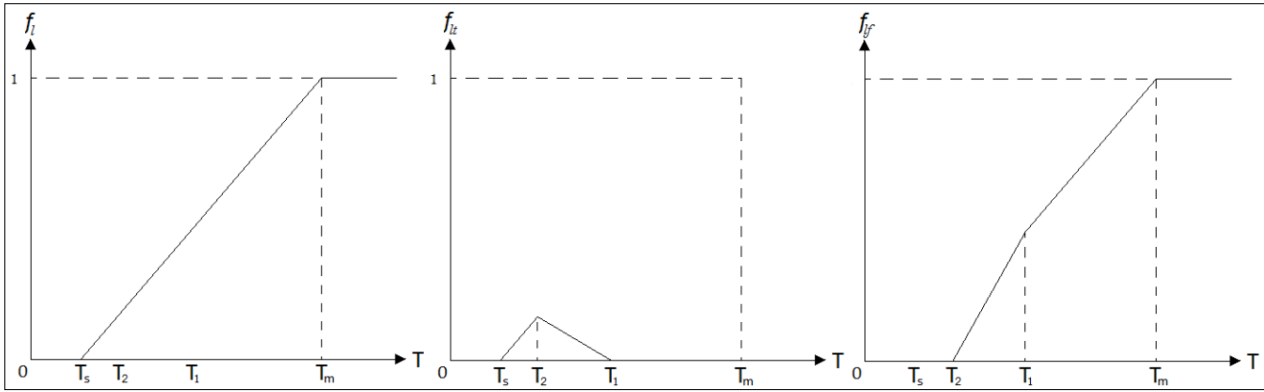

Figure 3 *Volume fraction of liquid vs. Temperature*

$$f_l = \frac{v_l}{v_l + v_s}$$ [7]A

$$f_{lt} = \frac{v_{lt}}{v_l + v_s}$$ [7]B

$$f_{lf} = \frac{v_{lf}}{v_l + v_s}$$ [7]C

where f_l is the volume fraction of all the liquid of the materials excluding the volume of the pores. Similarly, f_{lt} and f_{lf} are the volume fraction of trapped liquid and that of the free liquid, respectively. Notice that in **Figure 3**, f_{lt} and f_l coincide with each other from T_2 to T_s, whereas f_{lf} and f_l coincide with each other from T_m to T_1. Also, f_{lm} is the volume fraction of the free liquid of the matrix material i.e. solid and free liquid. Its significance is shown later in equation set [9].

$$f_{lm} = \frac{v_{lf}}{v_{lf} + v_s}$$ [7]D

Therefore a series of *if* statements can be prescribed as below

If $T \geq T_m$: $f_l = f_{lf} = f_{lm} = 1$, $f_{lt} = 0$

If $T_m > T > T_1$: $f_l = f_{lf} = f_{lm} = \frac{T-T_s}{T_m-T_s}$, $f_{lt} = 0$

If $T_1 \geq T > T_2$: $f_l = \frac{T-T_s}{T_m-T_s}$, $f_{lf} = f_l \frac{T-T_2}{T_1-T_2}$, $f_{lt} = f_l \frac{T_1-T}{T_1-T_2}$, $f_{lm} = \frac{f_{lf}}{1-f_{lt}}$

If $T_2 \geq T > T_s$: $f_l = f_{lt} = \frac{T-T_s}{T_m-T_s}$, $f_{lf} = f_{lm} = 0$

If $T_s \geq T$: $f_l = f_{lf} = f_{lt} = f_{lm} = 0$

ρ_l can then simply be derived from equation [3] and [7]B

$$\rho_l = \frac{v_{lt}}{V} = \frac{v_{lt}}{v_l + v_s} \cdot \frac{v_l + v_s}{V} = f_{lt}(1 - \rho_p) \tag{8}$$

Equation [8] along with the *if* statements can then be coded into the USER subroutine.

Also at temperature above T_2, there is always free liquid. Assume that there is an effective viscosity associated with the free liquid. This influence of the viscosity may be reflected in the reference strain rate $\dot{\varepsilon}_0$. Whilst both liquid and solid phases contribute to the materials response, liquid can be considered as a very soft solid, i.e. for a given temperature it creeps much more easily. If stresses are assumed to be the same in both phases, $\dot{\varepsilon}_0$ would vary linearly as follows

$$\dot{\varepsilon}_0 = f_{lm}\dot{\varepsilon}_{0l} + (1 - f_{lm})\dot{\varepsilon}_{0s} \tag{9]A}$$

where f_{lm} is the volume fraction of the free liquid of the matrix material (see equation [7]D), $\dot{\varepsilon}_{0l}$ is the reference strain rate when the material is completely liquid and $\dot{\varepsilon}_{0s}$ is the reference strain rate when the material is completely solid.

Alternatively, if the strain rate for both phases are assumed to be the same, $\dot{\varepsilon}_0$ would be

$$\dot{\varepsilon}_0 = \frac{\dot{\varepsilon}_{0s}}{\left[f_{lm} \left(\frac{\dot{\varepsilon}_{0s}}{\dot{\varepsilon}_{0l}} \right)^{1/n} + (1 - f_{lm}) \right]^n} \tag{9]B}$$

Either one of the equation set [9] can be coded into the USER subroutine.

abaqus integration scheme

As mentioned in the Introduction the implicit time integration scheme consists of defining the variation of the effective creep strain increment $\Delta\varepsilon^{cr}$ and volumetric strain increment $\Delta\varepsilon^{sw}$ with respect to σ_e and σ_m as shown below. Note that the Abaqus CREEP USER subroutine uses pressure $p\ (= -\sigma_m)$ instead of σ_m

$$\left(\frac{\partial \Delta\varepsilon^{cr}}{\partial \sigma_e} \right)_{-\sigma_m} = \left(\frac{\partial \dot{\varepsilon}_e dt}{\partial \sigma_e} \right)_{-\sigma_m}$$

$$= \dot{\varepsilon}_0 \left[(n-1) \left(\frac{\bar{\sigma}}{\sigma_0} \right)^{n-3} \frac{\sigma_e^2}{\sigma_0^3 g_2^2(\rho)} + \left(\frac{\bar{\sigma}}{\sigma_0} \right)^{n-1} \frac{1}{\sigma_0 g_2(\rho)} \right] exp \left[-\frac{Q}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] dt \tag{10]a}$$

$$+ \dot{\varepsilon}_p \left[(m-1) \left(\frac{\bar{\sigma}_p}{\sigma_p} \right)^{m-3} \frac{\sigma_e^2}{\sigma_p^3 g_{2p}^2(\rho)} + \left(\frac{\bar{\sigma}_p}{\sigma_p} \right)^{m-1} \frac{1}{\sigma_p g_{2p}(\rho)} \right] dt$$

$$\left(\frac{\partial \Delta\varepsilon^{cr}}{\partial(-\sigma_m)} \right)_{\sigma_e} = \left(\frac{\partial \dot{\varepsilon}_e dt}{\partial(-\sigma_m)} \right)_{\sigma_e} \tag{10]b}$$

$$= \dot{\varepsilon}_0 \left[(1-n) \left(\frac{\bar{\sigma}}{\sigma_0} \right)^{n-3} \frac{\sigma_m \sigma_e}{\sigma_0^3 g_2(\rho) g_3(\rho)} \right] exp \left[-\frac{Q}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] dt$$

$$+ \dot{\varepsilon}_p \left[(1-m) \left(\frac{\bar{\sigma}_p}{\sigma_p} \right)^{m-3} \frac{\sigma_m \sigma_e}{\sigma_p^3 g_{2p}(\rho) g_{3p}(\rho)} \right] dt$$

and

$$\left(\frac{\partial \Delta \varepsilon^{sw}}{\partial \sigma_e} \right)_{-\sigma_m} = \left(\frac{\partial \dot{\varepsilon}_v dt}{\partial \sigma_e} \right)_{-\sigma_m}$$

$$= \dot{\varepsilon}_0 \left[(n-1) \left(\frac{\bar{\sigma}}{\sigma_0} \right)^{n-3} \frac{\sigma_m \sigma_e}{\sigma_0^3 g_2(\rho) g_3(\rho)} \right] exp \left[-\frac{Q}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] dt \qquad [11]a$$

$$+ \dot{\varepsilon}_p \left[(m-1) \left(\frac{\bar{\sigma}_p}{\sigma_p} \right)^{m-3} \frac{\sigma_m \sigma_e}{\sigma_p^3 g_{2p}(\rho) g_{3p}(\rho)} \right] dt$$

$$\left(\frac{\partial \Delta \varepsilon^{sw}}{\partial (-\sigma_m)} \right)_{\sigma_e} = \left(\frac{\partial \dot{\varepsilon}_v dt}{\partial (-\sigma_m)} \right)_{\sigma_e}$$

$$= \dot{\varepsilon}_0 \left[(1-n) \left(\frac{\bar{\sigma}}{\sigma_0} \right)^{n-3} \frac{\sigma_m^2}{\sigma_0^3 g_3^2(\rho)} - \left(\frac{\bar{\sigma}}{\sigma_0} \right)^{n-1} \frac{1}{\sigma_0 g_3(\rho)} \right] exp \left[-\frac{Q}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] dt \qquad [11]b$$

$$+ \dot{\varepsilon}_p \left[(1-m) \left(\frac{\bar{\sigma}_p}{\sigma_p} \right)^{m-3} \frac{\sigma_m^2}{\sigma_p^3 g_{3p}^2(\rho)} - \left(\frac{\bar{\sigma}_p}{\sigma_p} \right)^{m-1} \frac{1}{\sigma_p g_{3p}(\rho)} \right] dt$$

Equation set [10] and [11] can be coded into the USER subroutine. Note that in this implicit integration scheme $g_2(\rho)$, $g_3(\rho)$, $g_{2p}(\rho)$ and $g_{3p}(\rho)$ are assumed to be constant over each increment, the only state variable ρ_p is updated with time independently at the end of each increment. This could either be achieved by using a simple Euler Scheme or by directly integrating from the volumetric strain rate for ρ_p as shown below:

by Euler Scheme

$$\rho_p^{t+\Delta t} = \rho_p^t + \dot{\rho}_p^t \Delta t$$

$$= \rho_p^t + \dot{\varepsilon}_v (1 - \rho_p) \Delta t \qquad [12]$$

by direct integration from equation [6]

$$\rho_p = 1 - exp(-\varepsilon_v) \qquad [13]A$$

It is recommended that for plotting purposes ρ_l be kept as the second state variable between temperature T_1 and T_2. From equation [8] and the *if* statements:

$$\rho_l = f_l \frac{T_1 - T}{T_1 - T_2} (1 - \rho_p) \qquad [13]B$$

Either equation [12] or [13]A as well as [13]B can then be used as the updating scheme for the state variables and be coded into the USER subroutine after equation set [10] and [11] (see creep_user_sub.for).