Model behavior élastovisqueuxMETA_LEMA_ANI with taking into account of the metallurgy for the tubes of sheath of the Summarized fuel pin

:

For the realization of computations 3D of the combustible sheath in accidental situation of type APRP, department MMC formulated, for the tubes in Zircaloy, a model of élastovisqueux behavior, without threshold, anisotropic and taking into account the effect of the transformation of phase alpha-beta on the structural mechanics behavior.

One describes this model, available here in *Code_Aster* under the name of `META_LEMA_ANI,` and his algorithm of resolution. It is available in 3D, plane strain, axisymetry.

The matrix of anisotropy of Hill is indicated in the cylindrical coordinate system associated with the tube. To date, it was supposed that the axial axis z of the cylindrical coordinate system associated with the tube corresponded to that of the total reference. So that if several tubes must be modelled or if the axis of the tube does not correspond to that of the total reference, the model is not correct. In the long term, this restriction would have to be raised.

The equations of velocity are integrated numerically by an implicit scheme of Eulerian. The system of equations obtained is solved by the method of Newton.

Contents

1 Context

At the time of the first phase of an accident of design of the type APRP (Accident of Primary education loss of Cooling agent), the fuel pins are subjected to a fast rise in temperature, transformations of phase of the material and to changes of mechanical boundary conditions. The study of an accident of APRP requires a good knowledge of the behavior of the sheath of the fuel pins at the time of the first phase known as of “swelling-fracture”. In particular, it is necessary to have a good idea of the total deflection of the sheath.

Models of transition from phases, structural mechanics behavior and fracture were developed, and identified on the basis of experimental test.

For the metallurgical part, sudden Zircaloy of the metallurgical transformations between 700°C and 1000°C, where they pass from a phase of compact hexagonal structure (cold phase alpha or α) to a cubic structure phase (hot phase beta or β). One will find in [R4.04.04], the equations governing the kinetics of the transformations to the heating (α is transformed into β) and to cooling (β is transformed into α).

For the mechanical part, the model is written into unidimensional, in the circumferential direction of the tube. Even if this model is in conformity with the experiments, its use to carry out computations with the finite elements 3D is not possible. Moreover, the zirconium alloys present an anisotropic behavior, at least in phase α, which cannot be taken into account in a model 1D. From a request point of view, the tube undergoes an azimuth variation in temperature involving of the deformation gradients circumferential, but as axial, as it is important to take into account to obtain a response in conformity with the experiment.

This is why, department MMC formulated a model 3D to describe the behavior of the sheath in Zircaloy in the case of a standard analysis APRP. The models of Norton describing the behavior 1D material in various fields $(\alpha, \alpha-\beta, \beta)$ are replaced by models of Lemaître, with taking into account of the anisotropy of the phase α . The phase β is isotropic. The formula $\alpha-\beta$ is supposed to have an anisotropy proportional to the presence rate of the phase α .

One describes here the establishment numerical of this model, available in *Code_Aster* under the name of `META_LEMA_ANI`, and his algorithm of resolution. It is available in 3D, plane strain, axisymetry.

2 Relation META_LEMA_ANI in *Code_Aster*

2.1 General information

The model presented is élastovisqueux, without threshold (the elastic limit is null), with taken into account of the metallurgical transformations of this material and taken into account of the anisotropy of the phase α. Viscosity is described by a model of the Lemaître type.

The model is introduced into *Code_Aster* in 3D, plane strains (D_PLAN), and axisymetry (AXIS) under the name of META_LEMA_ANI.

The taking into account of the anisotropy is carried out by a tensor of a nature 4 (matrix of Hill $\boldsymbol{M}$) affecting the models devolution of the viscous strain and the equivalent stress (von Mises stress within the meaning of Hill).

The equations of velocity are integrated numerically by an implicit scheme of Eulerian. The system obtained is solved by the method of Newton.

2.2 Restriction of use of the model

the equations of the model are written in the cylindrical coordinate system associated with the tube $(1=e_r, 2=e_\theta, 3=z)$. This is with the fact that the coefficients of the matrix of Hill, $\boldsymbol{M}$, are known in this reference.

On the level of the establishment in *Code_Aster*, one thus carries out a change of variables of the tensorial fields (another choice would have been to make undergo the change of variable to the tensor of Hill $\boldsymbol{M}$, but it is simpler to proceed contrary)

- For a computation 3D or into plane strain, the tensor of the stresses known in the total reference $(1=x, 2=y, 3=z)$ is transformed in the local coordinate system $(1=e_r, 2=e_\theta, 3=z)$;
- For a computation 2D, axisymmetric, the tensor of the stresses known in the total reference $(1=e_r, 2=z, 3=e_\theta)$ is calculated in the local coordinate system $(1=e_r, 2=e_\theta, 3=z)$; in this case, the change of variables is simple since it is only a question of inverting indices 2 and 3.

Limitation : it was supposed that on this axis of the cylindrical coordinate system z associated with the tube corresponded to that of the total reference. So that if several tubes must be modelled or if the axis of the tube does not correspond to that of the total reference, the model is not correct. In the long term, this restriction would have to be raised.

2.3 Use

1) the use of this model requires a preliminary computation of the proportions of the phases α and β, activated by the key word factor COMP_INCR=' ZIRC' of operator CALC_META.
2) In operator STAT_NON_LINE, one by means of reaches this mechanical model the key word following factor:

```
| COMP_INCR =  (
                  RELATION = “META_LEMA_ANI”
                  RELATION_KIT=' ZIRC'
                  ITER_INTE_MAXI = nombre of iterations maximum for Newton
```

RESI_INTE_RELA = stopping criteria of the process of Newton

3) the data materials relating to model META_LEMA_ANI, are indicated in operator DEFI_MATERIAU by means of the key keys factor ELAS_META and META_LEMA_ANI.

Note: the matrixes of Hill for the phases α and β are given in the cylindrical coordinate system $(1=e_r, 2=e_\theta, 3=z)$, even for a computation 2D axisymmetric where indices 2 and 3 are inverted.

2.4 Local variables

the local variables of model META_LEMA_ANI are:

$V1$: cumulated viscous strain
$V2$: the indicator of plasticity (0 or 1).

3 Notations

One will note by:

$\mathbf{Id}$	stamp identity
$Tr\,\mathbf{A}$	traces tensor $\mathbf{A}$
$\tilde{\mathbf{A}}$	deviatoric part of the tensor A definite by $\tilde{\mathbf{A}} = \mathbf{A} - (\frac{1}{3}\mathrm{Tr}\,\mathbf{A})\mathbf{Id}$
:	doubly contracted product: $\mathbf{A}:\mathbf{B} = \sum_{i,j} A_{ij}B_{ij} = \mathrm{Tr}(\mathbf{AB}^T)$
$\otimes$	tensor product: $(\mathbf{A}\otimes\mathbf{B})_{ijkl} = A_{ij}B_{kl}$
A_{eq}	equivalent value of Von Mises within the meaning of Hill defined by $A_{eq} = \sqrt{\mathbf{A}:\mathbf{M}:\mathbf{A}}$
$\mathbf{M}$	Matrix of anisotropy of Hill
λ , μ , E , ν , K	moduli of the isotropic elasticity
α	thermal coefficient of thermal expansion
T	temperature
T_{ref}	reference temperature

In addition, in the frame of a discretization in time, all the quantities evaluated at previous time are subscripted by $-$, the quantities evaluated at time $t+\Delta t$ are not subscripted and the increments are indicated par. Δ One has as follows:

$$\Delta Q = Q - Q^-$$

4 Presentation of model META_LEMA_ANI

4.1 important Remarks

- Thereafter, the equations of the model are presented in the cylindrical coordinate system $(\mathbf{1}=\mathbf{e_r}, \mathbf{2}=\mathbf{e_\theta}, \mathbf{3}=\mathbf{z})$, associated with the sheath of axis $\mathbf{z}$.
- From a purely metallurgical point of view, Zircaloy comprises two phases, the cold phase α and the hot phase β, which can be present simultaneously, by observing the condition $Z_\alpha + Z_\beta = 1$, where Z_α and Z_β the proportions of phase α and phase β represent, respectively.
- From a mechanical point of view, one considers, for materials parameters mechanical model, three phases: the phase 1 = pure phase α, the phase 2 = $\alpha\beta$ mixture and the phase 3 = pure phase β. This is why, one sees appearing three indices thereafter in the equations. The three phases are distinguished in the following way:
  - Si $0 \le Z_\alpha \le 0.01 =>$phase 3 = β
  - Si $0.01 \le Z_\alpha \le 0.1 =>$phases 3 = β et 2 = $\alpha\beta$ (loi des mélanges linéaire)
  - Si $0.1 \le Z_\alpha \le 0.9 =>$phase 2 = $\alpha\beta$
  - Si $0.9 \le Z_\alpha \le 0.99 =>$phases 1 = α et 2 = $\alpha\beta$ (loi des mélanges linéaire)
  - Si $0.99 \le Z_\alpha \le 1 =>$phase 1 = α

4.2 Equations of the model

the equations of the model are:

- Partition of the strains into cubes elastic parts $\boldsymbol{\varepsilon}^{\mathbf{e}}$, thermal $\varepsilon^{\mathrm{th}}$ and viscous $\boldsymbol{\varepsilon}^{\mathbf{v}}$:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\mathbf{e}} + \varepsilon^{\mathrm{th}}\,\mathbf{Id} + \boldsymbol{\varepsilon}^{\mathbf{v}} \quad \text{with} \quad \varepsilon^{\mathrm{th}} = \alpha(\mathrm{T} - T_{ref})$$

- Relation stress-strain: one separates the deviatoric part of the spherical part:

$$\boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \frac{1}{3}\sigma_{\mathrm{pp}}\mathbf{Id}$$

$$\sigma_{\mathrm{pp}} = 3K\left(\varepsilon_{\mathrm{pp}} - 3\,\varepsilon^{\mathrm{th}}\right)$$

$$\tilde{\boldsymbol{\sigma}} = 2\mu\left(\tilde{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}^{\mathbf{v}}\right)$$

- Flow models of the viscous strain:

$$\dot{\boldsymbol{\varepsilon}}^{\mathbf{v}} = \dot{\mathrm{p}}\frac{\mathbf{M}:\boldsymbol{\sigma}}{\sigma_{\mathrm{eq}}}$$

with the equivalent stress within the meaning of Hill defined by: $\sigma_{\mathrm{eq}} = \sqrt{\boldsymbol{\sigma}:\mathbf{M}:\boldsymbol{\sigma}}$

$$\mathbf{M} = \begin{cases} \mathbf{M^3} & \text{si } 0 \le Z_\alpha \le 0.01 \\ \mathbf{M^2} = Z_\alpha\,\mathbf{M^1} + (1\text{-}Z_\alpha)\mathbf{M^3} & \text{si } 0.01 \le Z_\alpha \le 0.99 \\ \mathbf{M}^1 & \text{si } 0.99 \le Z_\alpha \le 1 \end{cases}$$

The matrix of anisotropy of Hill, **M**, is form:

$$\mathbf{M}_{(\mathbf{e_r},\mathbf{e_\theta},\mathbf{z})}=\begin{bmatrix} M_{11} & M_{12} & M_{13} & 0 & 0 & 0\\ M_{12} & M_{22} & M_{23} & 0 & 0 & 0\\ M_{13} & M_{23} & M_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & M_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & M_{55} & 0\\ 0 & 0 & 0 & 0 & 0 & M66 \end{bmatrix} \text{avec} \begin{cases} M_{11}+M_{12}+M_{13}=0\\ M_{12}+M_{22}+M_{23}=0\\ M_{13}+M_{23}+M_{33}=0 \end{cases}$$

That is to say:

$$M_{12}=\frac{1}{2}\left(-M_{11}-M_{22}+M_{33}\right)$$
$$M_{13}=\frac{1}{2}\left(-M_{11}+M_{22}-M_{33}\right)$$
$$M_{23}=\frac{1}{2}\left(M_{11}-M_{22}-M_{33}\right)$$

Note: in the isotropic case, one a:

$$M_{11}=M_{22}=M_{33}=1$$
$$M_{12}=M_{13}=M_{23}=-\frac{1}{2}$$
$$M_{44}=M_{55}=M_{66}=\frac{3}{4}=0.75$$

- the equivalent strainrate is given by:

$$\dot{p}=\left(\frac{\sigma_{eq}}{ap^m}\right)^n e^{-Q/T} \text{ or in an equivalent way } \sigma_{eq}=\underbrace{a\left(e^{Q/T}\right)^{1/n} p^m \dot{p}^{1/n}}_{\text{contrainte visqueuse } \sigma_v}=\sigma_v$$

- Model of the mixtures on the viscous stress σ_v

$$\sigma_{eq}=\sigma_v=\sum_{i=1}^{3} f_i(Z_\alpha)\sigma_{vi} \text{ with } \sigma_{vi}=a_i\left(e^{Q_i/T}\right)^{1/n_i} p^{m_i}\dot{p}^{1/n_i}$$

$$f_1=\begin{cases} 0 & \text{si} \quad 0\le Z_\alpha\le 0.9\\ \dfrac{(Z_\alpha-0.9)}{0.09} & \text{si} \quad 0.9\le Z_\alpha\le 0.99\\ 1 & \text{si} \quad 0.99\le Z_\alpha\le 1 \end{cases},\qquad f_3=\begin{cases} 1 & \text{si} \quad 0\le Z_\alpha\le 0.01\\ \dfrac{(0.1-Z_\alpha)}{0.09} & \text{si} \quad 0.01\le Z_\alpha\le 0.1\\ 0 & \text{si} \quad 0.1\le Z_\alpha\le 1 \end{cases}$$

$$f_2 = \begin{cases} 0 & \text{si} \quad 0 \le Z_\alpha \le 0.01 \\ 1 - \dfrac{(0.1 - Z_\alpha)}{0.09} & \text{si} \quad 0.01 \le Z_\alpha \le 0.1 \\ 1 & \text{si} \quad 0.1 \le Z_\alpha \le 0.9 \\ 1 - \dfrac{(Z_\alpha - 0.9)}{0.09} & \text{si} \quad 0.9 \le Z_\alpha \le 0.99 \\ 0 & \text{si} \quad 0.99 \le Z_\alpha \le 1 \end{cases}$$

where (a_i, Q_i, n_i, m_i) are materials parameters attached to the three metallurgical phases.

5 Integration of the model

5.1 Discretization of the equations

Knowing the tensor of the stresses $\boldsymbol{\sigma}^-$, the equivalent viscous strain p^-, the tensors of the total deflections $\boldsymbol{\varepsilon}^-$ and $\Delta\boldsymbol{\varepsilon}$, temperatures T^- and T, and the proportion of phase α Z_α, one seeks to determine $(\boldsymbol{\sigma}, p)$.

The implicit discretization of the model gives:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\mathbf{e}} + \varepsilon^{th}\mathbf{Id} + \boldsymbol{\varepsilon}^{\mathbf{v}} \text{ with } \varepsilon^{th} = \alpha(T - T_{ref}) \quad \textbf{éq. 5.1-1}$$

$$\boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \frac{1}{3}\mathrm{Tr}\,\boldsymbol{\sigma}\,\mathbf{Id} \quad \textbf{éq. 5.1-2}$$

$$\mathrm{Tr}\,\boldsymbol{\sigma} = 3K\left(\mathrm{Tr}\,\boldsymbol{\varepsilon} - 3\varepsilon^{th}\right) \quad \textbf{éq. 5.1-3}$$

$$\tilde{\boldsymbol{\sigma}} = 2\mu\left(\tilde{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}^{\mathbf{v}}\right) \quad \textbf{éq. 5.1-4}$$

$$\Delta\boldsymbol{\varepsilon}^{\mathbf{v}} = \Delta p \frac{\mathbf{M}:\boldsymbol{\sigma}}{\sigma_{eq}} \quad \textbf{éq. 5.1-5}$$

$$\sigma_{eq} = \sqrt{\boldsymbol{\sigma}:\mathbf{M}:\boldsymbol{\sigma}} \quad \textbf{éq. 5.1-6}$$

$$\sigma_{eq} = \sum_{i=1}^{3} f_i(Z_\alpha) a_i \left(e^{Q_i/T}\right)^{1/n_i} \left(p^- + \Delta p\right)^{m_i} \left(\frac{\Delta p}{\Delta t}\right)^{1/n_i} \quad \textbf{éq. 5.1-7}$$

In the resolution of this system, only the deviatoric stress $\tilde{\boldsymbol{\sigma}}$ is unknown because the trace of $\boldsymbol{\sigma}$ is function only deflections total $\boldsymbol{\varepsilon}$ and thermal ε^{th}, which are known.

While replacing in equation 5.1-5, the tensor of the viscous strains according to the stress tensor deviatoric drawn from equation 5.1-4, one obtains finally the following system:

$$\tilde{\boldsymbol{\sigma}} + 2\mu\Delta p \frac{\mathbf{M}:\boldsymbol{\sigma}}{\sigma_{eq}} = \underbrace{2\mu\Delta\tilde{\varepsilon} + \frac{2\mu}{2\mu^-}\tilde{\boldsymbol{\sigma}}^-}_{\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}} = \tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}} \quad \textbf{éq. 5.1-8}$$

$$\sigma_{eq} = \sqrt{\boldsymbol{\sigma}:\mathbf{M}:\boldsymbol{\sigma}} \quad \textbf{éq. 5.1-9}$$

$$\sigma_{eq} = \sum_{i=1}^{3} f_i(Z_\alpha) a_i \left(e^{Q_i/T}\right)^{1/n_i} \left(p^- + \Delta p\right)^{m_i} \left(\frac{\Delta p}{\Delta t}\right)^{1/n_i} \quad \textbf{éq. 5.1-10}$$

the tensor of the stresses $\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}$ is known since it is function of the increment of the tensor of the total deflections and the tensor of the stresses at previous time.
The resolution of this system of equations, whose unknowns are $\left(\tilde{\boldsymbol{\sigma}}, \sigma_{eq}, \Delta p\right)$, is made in *the Code_Aster* by a method of Newton.

Once solved this system, one from of deduced the tensor from the stresses $\boldsymbol{\sigma}$ and the equivalent strain p :

$$\boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + K\left[\mathrm{Tr}\left(\boldsymbol{\varepsilon}^- + \Delta\boldsymbol{\varepsilon}\right) - 3\alpha\left(T - T_{ref}\right)\right]\mathbf{Id}$$ **éq. 5.1-11**

$$p = p^- + \Delta p$$ **éq. 5.1-12**

5.2 Resolution

Thereafter, one will pose:

$$\tilde{\boldsymbol{\sigma}} = 2\mu\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}$$ **éq. 5.2-1**

$$N_i = \frac{1}{n_i}$$ **éq. 5.2-2**

$$\gamma_i = \frac{1}{2\mu} f_i(Z_\alpha) a_i \frac{e^{N_i Q_i / T}}{\Delta t^{N_i}}$$ **éq. 5.2-3**

system 5.1-8 to 5.1-10 is written in stress:

$$\mathbf{C}^{\mathbf{1}}(\tilde{\boldsymbol{\sigma}}, \Delta p) = \tilde{\boldsymbol{\sigma}} + 2\mu\Delta p \frac{\mathbf{M} : \boldsymbol{\sigma}}{\sqrt{\boldsymbol{\sigma} : \mathbf{M} : \boldsymbol{\sigma}}} - \tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}} = 0$$ **éq. 5.2-4**

$$C^2(\boldsymbol{\sigma}, \Delta p) = \sqrt{\boldsymbol{\sigma} : \mathbf{M} : \boldsymbol{\sigma}} - 2\mu \sum_{i=1}^{3} \gamma_i \left(p^- + \Delta p\right)^{m_i} \Delta p^{N_i} = 0$$ **éq. 5.2-5**

to facilitate the method of Newton, it is preferable to choose unknowns in the same unit (thus either of the stresses, or of the strains). One will use for that the relation 5.2-1 between the tensor of the stresses and the tensor of the elastic strain $\tilde{\varepsilon}_{ij}^{e}$ which becomes the unknown of the problem then (what has the advantage of adimensionnaliser the system). Finally, the system to be solved is written:

$$G^{\mathbf{1}}(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}, \Delta p) = \frac{C^{\mathbf{1}}}{2\mu} = \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \Delta p \frac{\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\sqrt{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}} - \frac{\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}}{2\mu} = 0$$ **éq. 5.2-6**

$$G^2(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}, \Delta p) = \frac{C^2}{2\mu} = \sqrt{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}} - \sum_{i=1}^{3} \gamma_i \left(p^- + \Delta p\right)^{m_i} \Delta p^{N_i} = 0$$ **éq. 5.2-7**

In more contracted way, one poses:

$$\mathbf{G}(\mathbf{y}) = \mathbf{0} = \begin{bmatrix} \mathbf{G}^{\mathbf{1}}(\mathbf{y}) \\ G^2(\mathbf{y}) \end{bmatrix} \text{ avec } \mathbf{y} = \begin{bmatrix} \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} \\ \Delta p \end{bmatrix}$$ **éq. 5.2-8**

the resolution by the method of Newton gives:

$$\begin{cases} \dfrac{\partial \mathbf{G}(\mathbf{y_n})}{\partial \mathbf{y}} \delta\mathbf{y_n} = -\mathbf{G}(\mathbf{y_n}) \\ \mathbf{y_{n+1}} = \mathbf{y_n} + \delta\mathbf{y_n} \end{cases}$$ **éq. 5.2-9**

While reiterating in n until convergence.

One gives the form of the tensor $\frac{\partial \mathbf{G}}{\partial \mathbf{y}}$ hereafter: computations are specified in appendix 1 (in the appendix the statements are given in indicielle form).

$$\frac{\partial \mathbf{G}}{\partial \mathbf{y}}=\begin{bmatrix} \frac{\partial \mathbf{G^1}}{\partial \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}} & \frac{\partial \mathbf{G^1}}{\partial \Delta p} \\ \frac{\partial G^2}{\partial \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}} & \frac{\partial G^2}{\partial \Delta p} \end{bmatrix} \quad \text{éq. 5.2-10}$$

Where each term is worth:

$$\frac{\partial \mathbf{G^1}}{\partial \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}=\mathbf{C}+\frac{\Delta p}{\varepsilon^e_{eq}}\mathbf{M}-\frac{\Delta p}{\left(\varepsilon^e_{eq}\right)^3}(\mathbf{M}:\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}})\otimes(\mathbf{M}:\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}})\ ;\ \frac{\partial \mathbf{G^1}}{\partial \Delta p}=\frac{1}{\varepsilon^e_{eq}}\mathbf{M}:\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} \quad \text{éq. 5.2-11}$$

$$\frac{\partial G^2}{\partial \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}=\frac{\mathbf{M}:\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\varepsilon^e_{eq}}\ ;\ \frac{\partial G^2}{\partial \Delta p}=-\sum_{i=1}^{3}\gamma_i\left(p^-+\Delta p\right)^{m_i}\Delta p^{N_i}\left(\frac{N_i}{\Delta p}+\frac{m_i}{p^-+\Delta p}\right) \quad \text{éq. 5.2-12}$$

With $C_{ijkl}=\frac{1}{2}\left(\delta_{ik}\delta_{jl}+\delta_{jk}\delta_{il}\right)$

5.2.1 Algorithm

1) So $\sigma^{Tr}_{eq}=0$ then $\tilde{\boldsymbol{\sigma}}=\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}$ et $p=p^-$
2) If not

2.1) Initialization of the method of Newton: solution for M isotropic

$$\tilde{\boldsymbol{\sigma}}+3\mu\Delta p\frac{\tilde{\boldsymbol{\sigma}}}{\sigma_{eq}}-\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}=0\Leftrightarrow\tilde{\boldsymbol{\sigma}}\left(1+3\mu\frac{\Delta p}{\sigma_{eq}}\right)=\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}} \quad \text{éq. 5.2.1-1}$$

$$\Leftrightarrow \sigma_{eq}=\sigma^{Tr}_{eq}-3\mu\Delta p$$

$$\sigma^{Tr}_{eq}-3\mu\Delta p=2\mu\sum_{i=1}^{3}\gamma_i\left(p^-+\Delta p\right)^{m_i}\Delta p^{N_i} \quad \text{éq. 5.2.1-2}$$

Once Δp known (by the algorithm describes with the § 5.2.2), one from of deduced σ_{eq} and $\tilde{\boldsymbol{\sigma}}$ which is used for the initialization as Newton

2.2) Iteration of Newton

the iterative process stops when the maximum of function **G (there)** is lower or equal to the criterion given by the user (key word RESI_INTE_RELA under COMP_INCR of operator STAT_NON_LINE). If the nombre of iterations exceeds that given by the user, the process stops in fatal error.

3) Computation of the tangent matrix

5.2.2 Resolution of the isotropic problem

One must solve the following equation:

$$\sigma_{eq}^{Tr} - 3\mu\Delta p = 2\mu\sum_{i=1}^{3}\gamma_i\left(p^- + \Delta p\right)^{m_i}\Delta p^{N_i}$$ **éq. 5.2.2-1**

One will pose thereafter $\Delta p = x \geq 0$.

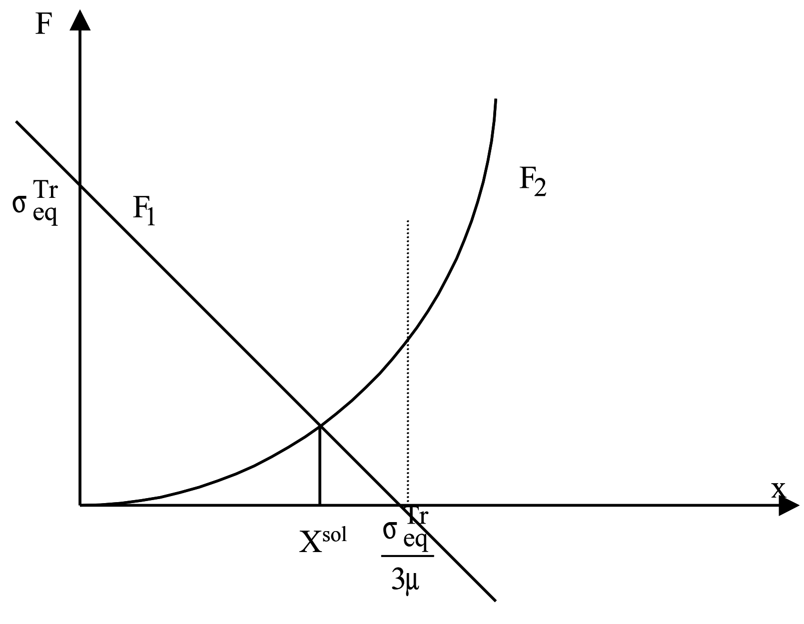
One also poses:

$$F_1(x) = \sigma_{eq}^{Tr} - 3\mu x \Rightarrow F_1'(x) = -3\mu \leq 0 \quad \forall x$$ **éq. 5.2.2-2**

And

$$F^2(x) = 2\mu\sum_{i=1}^{3}\gamma_i\left(p^- + x\right)^{m_i} x^{N_i}$$
$$F^{2'}(x) = 2\mu\sum_{i=1}^{3}\gamma_i\left[m_i\left(p^- + x\right)^{m_i - 1} x^{N_i} + N_i\left(p^- + x\right)^{m_i} x^{N_i - 1}\right]$$ **éq. 5.2.2-3**

the function $F_1(x)$ is a decreasing linear function in x. The function $F_2(x)$ is an increasing positive function in x. The solution X^{sol} is limited enters 0 and $\frac{\sigma_{eq}^{Tr}}{3\mu}$. One solves equation 5.3.2-1 by a method of Newton with controlled limit. The initialization of Newton will be done with the higher limit $\frac{\sigma_{eq}^{Tr}}{3\mu}$.



The method of Newton gives:

$$F(x) = F^1(x) - F^2(x) = \sigma_{eq}^{Tr} - 3\mu x - 2\mu \sum_{i=1}^{3} \gamma_i \left(p^- + x\right)^{m_i} x^{N_i}$$

$$x^{k+1} = x^k - \frac{F(x^k)}{F'(x^k)}$$ **éq. 5.2.2-4**

Is:

$$x^{k+1} = x^k - \frac{\left[\sigma_{eq}^{Tr} - 3\mu x^k - 2\mu \sum_{i=1}^{3} \gamma_i \left(p^- + x^k\right)^{m_i} x^{k^{N_i}}\right]}{\left[-3\mu - 2\mu \sum_{i=1}^{3} \gamma_i \left[m_i \left(p^- + x^k\right)^{m_i - 1} x^{N_i} + N_i \left(p^- + x^k\right)^{m_i} x^{k^{N_i - 1}}\right]\right]}$$ **éq. 5.2.2-5**

5.3 Form of the tangent matrix

the formed system by the equations of the model written in discretized form $(\mathbf{G}(\mathbf{y}) = 0)$ is checked at the end of the increment. For a small variation of $\mathbf{G}$, by regarding this time $\Delta\boldsymbol{\varepsilon}$ variable and not as parameter, the system remains with the equilibrium and one checks $\mathrm{d}\mathbf{G} = \mathbf{0}$, i.e.:

$$\begin{bmatrix} \frac{\partial \mathbf{G^1}}{\partial \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}} & \frac{\partial \mathbf{G^1}}{\partial \Delta p} \\ \frac{\partial G^2}{\partial \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}} & \frac{\partial G^2}{\partial \Delta p} \end{bmatrix} \begin{bmatrix} \delta \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} \\ \delta \Delta p \end{bmatrix} = \begin{bmatrix} \delta \Delta \tilde{\boldsymbol{\varepsilon}} \\ 0 \end{bmatrix}$$ **éq. 5.3-1**

the preceding equations show that one is led to re-use the same matrix $\frac{\partial \mathbf{G}}{\partial \mathbf{y}}$ as previously to evaluate the tangent operator.
It is obviously necessary to supplement by the part traces. One can with final writing the tangent matrix **H** as follows:

$$\delta \sigma_{ij} = H_{ijkl}\, \delta \Delta \varepsilon_{kl},\ D_{ijkl} = \left(\frac{\partial \mathbf{G}}{\partial \mathbf{y}}\right)^{-1}_{ijkl}$$

$$H_{ijkl} = 2\mu D_{ijkl} + \frac{1}{3}\left(2\mu D_{ijpp} + 3K \delta_{ij}\right)\delta_{kl}$$ **éq. 5.3-1**

6 Description of the versions

Index document	**Version Aster**	**Author (S) Organization (S)**	**Description of the modifications**
A	9.4	V.Cano, R & D AMA	initial Text

Annexe 1 : Statement of the Jacobian

In order to obtain the tensor $\frac{\partial \mathbf{G}}{\partial \mathbf{y}}$ which will be useful for the resolution of Newton, it is enough to linearize each statement below:

$$\mathbf{G^1} = \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \Delta p \frac{\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\sqrt{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}} - \frac{\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}}{2\mu} \qquad \text{éq. A1-1}$$

$$G^2 = \sqrt{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}} - \sum_{i=1}^{3} \gamma_i \left(p^- + \Delta p\right)^{m_i} \Delta p^{1/n_i} \qquad \text{éq. A1-2}$$

•**Linearization of the A1-1 equation:**

$$\mathbf{G^1} + \delta\mathbf{G^1} = \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + (\Delta p + \delta\Delta p) \frac{\mathbf{M} : \left(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\right)}{\sqrt{\left(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\right) : \mathbf{M} : \left(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\right)}} - \frac{1}{2\mu}\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}$$

$$\Leftrightarrow \mathbf{G^1} + \delta\mathbf{G^1} = \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \frac{(\Delta p + \delta\Delta p)\mathbf{M} : \left(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\right)}{\sqrt{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + 2\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}} - \frac{1}{2\mu}\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}$$

$$\Leftrightarrow \mathbf{G^1} + \delta\mathbf{G^1} = \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \frac{1}{\varepsilon_{eq}^{e}}(\Delta p + \delta\Delta p)\mathbf{M} : \left(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\right)\left(1 - \frac{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\varepsilon_{eq}^{2e}}\right) - \frac{1}{2\mu}\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}$$

$$\Leftrightarrow \mathbf{G^1} + \delta\mathbf{G^1} = \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \frac{1}{\varepsilon_{eq}^{e}}\left(\Delta p\,\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \Delta p\,\mathbf{M} : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\Delta p\,\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\right)\left(1 - \frac{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\varepsilon_{eq}^{2e}}\right) - \frac{1}{2\mu}\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}$$

$$\Leftrightarrow \mathbf{G^1} + \delta\mathbf{G^1} = \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \frac{1}{\varepsilon_{eq}^{e}}\left(\Delta p\,\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \Delta p\,\mathbf{M} : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\,\delta\Delta p - \Delta p\,\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\,\frac{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\varepsilon_{eq}^{2e}}\right) - \frac{1}{2\mu}\tilde{\boldsymbol{\sigma}}^{\mathbf{Tr}}$$

$$\Leftrightarrow \delta\mathbf{G^1} = \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \frac{1}{\varepsilon_{eq}^{e}}\left(\Delta p\,\mathbf{M} : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\,\delta\Delta p - \Delta p\,\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\,\frac{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M} : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\varepsilon_{eq}^{2e}}\right)$$

$$\Leftrightarrow \delta\mathbf{G^1} = \left(\mathbf{C} + \frac{\Delta p}{\varepsilon_{eq}^{e}}\mathbf{M} - \frac{\Delta p}{\varepsilon_{eq}^{3e}}(\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}) \otimes (\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} : \mathbf{M})\right) : \delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}} + \frac{1}{\varepsilon_{eq}^{e}}\mathbf{M} : \tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\,\delta\Delta p$$

from where in indicielle form:

$$\frac{\partial G_{ij}^{1}}{\partial \tilde{\varepsilon}_{kl}^{e}} = C_{ijkl} + \frac{\Delta p}{\varepsilon_{eq}^{e}} M_{ijkl} - \frac{\Delta p}{\varepsilon_{eq}^{3e}} M_{ijpq}\,\tilde{\varepsilon}_{pq}^{e}\,\tilde{\varepsilon}_{rs}^{e} M_{rskl}\ ;\quad \frac{\partial G_{ij}^{1}}{\partial \Delta p} = \frac{1}{\varepsilon_{eq}^{e}} M_{ijkl}\,\tilde{\varepsilon}_{kl}^{e}$$

with $C_{ijkl} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{jk}\delta_{il}\right)$

- **Linearization of the A1-2 equation:**

$$G^2+\delta G^2=\sqrt{\left(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}+\delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\right):\mathbf{M}:\left(\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}+\delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}\right)}-\sum_{i=1}^{3}\gamma_i\left(p^-+\Delta p+\delta\Delta p\right)^{m_i}\left(\Delta p+\delta\Delta p\right)^{1/n_i}$$

$$\Leftrightarrow G^2+\delta G^2=\sqrt{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}:\mathbf{M}:\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}+2\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}:\mathbf{M}:\delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}-\sum_{i=1}^{3}\gamma_i\left(p^-+\Delta p\right)^{m_i}\left(1+\frac{\delta\Delta p}{p^-+\Delta p}\right)^{m_i}\Delta p^{1/n_i}\left(1+\frac{\delta\Delta p}{\Delta p}\right)^{1/n_i}$$

$$\Leftrightarrow G^2+\delta G^2\cong\sqrt{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}:\mathbf{M}:\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}(1+\frac{2\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}:\mathbf{M}:\delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}:\mathbf{M}:\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}})}-\sum_{i=1}^{3}\gamma_i\left(p^-+\Delta p\right)^{m_i}\left(1+\frac{m_i\delta\Delta p}{p^-+\Delta p}\right)\Delta p^{1/n_i}\left(1+\frac{\delta\Delta p}{n_i\Delta p}\right)$$

$$\Leftrightarrow G^2+\delta G^2\cong\varepsilon_{eq}^{e}(1+\frac{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}:\mathbf{M}:\delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\varepsilon_{eq}^{2e}})-\sum_{i=1}^{3}\gamma_i\left(p^-+\Delta p\right)^{m_i}\Delta p^{1/n_i}\left(1+\frac{\delta\Delta p}{n_i\Delta p}+\frac{m_i\delta\Delta p}{p^-+\Delta p}\right)$$

$$\Leftrightarrow \delta G^2\cong\frac{\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}:\mathbf{M}:\delta\tilde{\boldsymbol{\varepsilon}}^{\mathbf{e}}}{\varepsilon_{eq}^{e}}-\sum_{i=1}^{3}\gamma_i\left(p^-+\Delta p\right)^{m_i}\Delta p^{1/n_i}\left(\frac{1}{n_i\Delta p}+\frac{m_i}{p^-+\Delta p}\right)\delta\Delta p$$

from where

$$\frac{\partial G^2}{\partial\tilde{\varepsilon}_{kl}^{e}}=\frac{\tilde{\varepsilon}_{ij}^{e}M_{ijkl}}{\varepsilon_{eq}^{e}}\;;\quad\frac{\partial G^2}{\partial\Delta p}=-\sum_{i=1}^{3}\gamma_i\left(p^-+\Delta p\right)^{m_i}\Delta p^{1/n_i}\left(\frac{1}{n_i\Delta p}+\frac{m_i}{p^-+\Delta p}\right)$$