Model of élasto-viscous behavior `META_LEMA_ANI` with taking into account of the metallurgy for the tubes of sheath of the fuel pin

Summary:

For the realization of calculations 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 fascinating of account the effect of the transformation of phase alpha-beta on the mechanical behavior.

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

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

The equations of speed are integrated numerically by an implicit scheme of Euler. 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 dimensioning 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 material and to changes of boundary conditions mechanical. 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-rupture”. In particular, it is necessary to have a good idea of the total deflection of the sheath.

models of transition from phases, mechanical behavior and rupture were developed, and identified on the basis of experimental test.

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

For the mechanical part, the model is written into unidimensional, in the direction circumferential of the tube. Even if this model is in conformity with the experiments, its use to carry out calculations 3D with the finite elements 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 gradients of deformation circumferential, but as axial, as it is important to take into account to obtain an answer in conformity with the experiment.

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

One describes here the digital establishment of this model, available in *Code_hasster* under the name of `META_LEMA_ANI`, and its algorithm of resolution. It is available in 3D, plane deformation, axisymetry.

2 Relation META_LEMA_ANI in *Code_Aster*

2.1 General information

The model presented is élastovisqueux, without threshold (the elastic limit is worthless), with taken into account of the metallurgical transformations of this material (described in the R4.04.04 document) and taken into account of the anisotropy of the phase. Viscosity is described by a law of the Lemaître type.

The model is introduced into *Code_Aster* in 3D, plane deformations (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 order 4 (matrix of Hill $\boldsymbol{M}$) affecting the laws devolution of the viscous deformation and the equivalent constraint (forced of Von Mises within the meaning of Hill).

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

2.2 Restriction of use of the model

The equations of the model can be written either in coordinates Cartesian, that is to say in the cylindrical reference mark associated with the tube $(1=e_r, 2=e_\theta, 3=z)$. This is Dû with the fact that coefficients of the matrix of Hill, $\boldsymbol{M}$, are known in this reference mark.

On the level of the establishment in *Code_hasster*, one carries out in this case 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 calculation 3D or in plane deformation, the tensor of the constraints known in the total reference mark $(1=x, 2=y, 3=z)$ is transformed in the local reference mark $(1=e_r, 2=e_\theta, 3=z)$;
- For a calculation 2D, axisymmetric, the tensor of the constraints known in the total reference mark $(1=e_r, 2=z, 3=e_\theta)$ is calculated in the local reference mark $(1=e_r, 2=e_\theta, 3=z)$; 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 the axis z cylindrical reference mark associated with the tube corresponded to that of the total reference mark. SI several tubes must be modelled or if the axis of the tube does not correspond to that of the total reference mark, it is to date necessary to use a script capitalized in the case test hsnv134b to take into account this difference.

2.3 Use

In the operator STAT_NON_LINE, one reaches this mechanical model by using the keyword RELATION = 'META_LEMA_ANI' in the keyword factor BEHAVIOR.
Lbe given materials relating to the model META_LEMA_ANI are well informed in the operator DEFI_MATERIAU by using the keywords factor META_LEMA_ANI.

Notice : **matrices of Hill for the phases α and β are given in the cylindrical reference mark $(1=e_r, 2=e_\theta, 3=z)$, even for an axisymmetric calculation 2D where indices 2 and 3 are inverted.**

2.4 Internal variables

Internal variables of the model META_LEMA_ANI are:

$V1 \rightarrow VN$: components of the tensor symmetrical elastic strain (N is worth 6 in 3D and 4 in 2D)
$VN+1$: cumulated viscous deformation p

$VN+2$: proportion of beta phase Z_{β}
$VN+3$: thermal deformation ε^{th}
$VN+4$: equivalent constraint of Hill A_{eq}
$VN+5,+6,+7$: constraintS viscousS σ_{v1} , σ_{v2} and σ_{v3} , respectively phases α pure, $\alpha\beta$ and β
$VN+8$: indicator of phase shift (0 or 1)
$VN+9$: moment to which the temperature is worth TDEQ (initialized to 0 at the beginning of calculation)
$VN+10$: moment to which the temperature is worth TFEQ (initialized to 0 at the beginning of calculation)

3 Notations

One will note by:

$\mathbf{Id}$	matrix identity
$Tr\,\mathbf{A}$	trace of the tensor $\mathbf{A}$
$\tilde{A}$	deviatoric part of the tensor A defined by $\tilde{\mathbf{A}}=\mathbf{A}-(\frac{1}{3}\mathrm{Tr}\,\mathbf{A})\mathbf{Id}$
:	doubly contracted product: $\mathbf{A}:\mathbf{B}=\sum_{i,j}A_{ij}B_{ij}=\mathrm{Tr}(\mathbf{AB}^T)$
$\otimes$	tensorial 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 dilation coefficient
T	temperature
T_{ref}	temperature of reference

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

$$\Delta Q=Q-Q^{-} \quad (1)$$

4 Presentation of the model META_LEMA_ANI

Thereafter, the equations of the model are presented in a "generic" reference mark (1,2,3) which represents either the Cartesian reference mark (OX, OY, OZ), or the cylindrical reference mark $(1=e_r, 2=e_\theta, 3=z)$ associated with the sheath of axis z .

4.1 Metallurgical phases

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 represent of phase α and of phase β , respectively.
From a mechanical point of view, one considers, for the parameters materials of the mechanical model, three phases: the phase 1 = phase α pure, the phase 2 = mixture $\alpha\beta$ and the phase 3 = phase β pure. This is why, one sees appearing three indices thereafter in the equations. The three phases are distinguished in the following way:

- If $0 \le Z_\alpha \le 0{,}01$ then phase 3 is the phase β
- If $0{,}01 \le Z_\alpha \le 0{,}1$ then phase 3 is the phase β and phase 2 is the mixed phase $\alpha\beta$ (linear law of the mixtures)
- If $0{,}1 \le Z_\alpha \le 0{,}9$ then phase 2 is the mixed phase $\alpha\beta$
- If $0{,}9 \le Z_\alpha \le 0{,}99$ then phase 1 is the phase α and phase 2 is the mixed phase $\alpha\beta$ (linear law of the mixtures)
- If $0{,}99 \le Z_\alpha \le 1{,}00$ then phase 1 is the phase α

4.2 Equations of the model

One carries out the partition of the deformations into cubes rubber band parts $\boldsymbol{\varepsilon}^e$, thermics ε^{th} and viscous $\boldsymbol{\varepsilon}^v$:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \varepsilon^{th} \boldsymbol{Id} + \boldsymbol{\varepsilon}^v \quad \text{with} \quad \varepsilon^{th} = \alpha (T - T_{ref}) \tag{2}$$

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

$$\boldsymbol{\sigma} = \tilde{\boldsymbol{\sigma}} + \frac{1}{3} \sigma_{pp} \boldsymbol{Id} \quad \text{With} \quad \sigma_{pp} = 3K \left(\varepsilon_{pp} - 3\varepsilon^{th} \right) \tag{3}$$

And one a:

$$\tilde{\boldsymbol{\sigma}} = 2\mu \left(\tilde{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}^v \right) \tag{4}$$

With the law of flow of the viscous deformation such as:

$$\dot{\boldsymbol{\varepsilon}}^v = \dot{p} \frac{\boldsymbol{M} : \boldsymbol{\sigma}}{\sigma_{eq}} \tag{5}$$

with the equivalent constraint within the meaning of Hill defined by:

$$\sigma_{eq} = \sqrt{\boldsymbol{\sigma} : \boldsymbol{M} : \boldsymbol{\sigma}} \tag{6}$$

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

$$\boldsymbol{M}_{(\boldsymbol{e}_r, \boldsymbol{e}_\theta, \boldsymbol{e}_z)} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & 0 & 0 & 0 \\ M_{12} & M_{22} & M_{23} & 0 & 0 & 0 \\ M_{13} & M_{23} & M_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & M_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & M_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & M_{66} \end{bmatrix} \quad \text{with} \quad \begin{cases} M_{11} + M_{12} + M_{13} + 0 \\ M_{12} + M_{22} + M_{23} + 0 \\ M_{13} + M_{23} + M_{33} + 0 \end{cases} \tag{7}$$

With:

$$\begin{cases} M_{11}+M_{12}+M_{13}+0 \\ M_{12}+M_{22}+M_{23}+0 \\ M_{13}+M_{23}+M_{33}+0 \end{cases} \text{ and thus } \begin{cases} M_{12}=\frac{1}{2}\left(-M_{11}-M_{22}+M_{33}\right) \\ M_{13}=\frac{1}{2}\left(-M_{11}+M_{22}-M_{33}\right) \\ M_{23}=\frac{1}{2}\left(M_{11}-M\,22-M_{33}\right) \end{cases} \tag{8}$$

In the isotropic case, one a:

$$\begin{gathered} M_{11}=M_{22}=M_{33}=1 \\ M_{12}=M_{13}=M_{23}=-\frac{1}{2} \\ M_{44}=M_{55}=M_{66}=\frac{3}{4} \end{gathered} \tag{9}$$

The terms of this matrices depend on the distribution in phase, with:

$$\boldsymbol{M}=\begin{cases} \boldsymbol{M}^3 \text{ si } 0\le Z_\alpha\le 0{,}01 \\ \boldsymbol{M}^2=Z_\alpha \boldsymbol{M}^1+\left(1-Z_\alpha\right)\boldsymbol{M}^3 \text{ si } 0{,}01\le Z_\alpha\le 0{,}99 \\ \boldsymbol{M}^1 \text{ si } 0{,}99\le Z_\alpha\le 1 \end{cases} \tag{10}$$

The speed of equivalent deformation is given by:

$$\dot{p}=\left(\frac{\sigma_{eq}}{a p^m}\right)^n e^{-Q/T} \tag{11}$$

Or in an equivalent way:

$$\sigma_{eq}=a\left(e^{Q/T}\right)^{1/n} p^m \dot{p}^{1/n}=\sigma_v \tag{12}$$

The L is appliedoi of the mixtures on the viscous constraint σ_v :

$$\sigma_{eq}=\sigma_v=\sum_{i=1}^{3} f_i\left(Z_\alpha\right)\sigma_{v,i} \text{ with } \sigma_{v,i}=a\left(e^{Q_i/T}\right)^{1/n_i} p^{m_i} \dot{p}^{1/n_i} \tag{13}$$

With:

$$\begin{gathered} f_1=\begin{cases} 0 \text{ si } 0\le Z_\alpha\le 0{,}9 \\ \frac{Z_\alpha-0{,}9}{0{,}09} \text{ si } 0{,}9\le Z_\alpha\le 0{,}99 \\ 1 \text{ si } 0{,}99\le Z_\alpha\le 1 \end{cases} \\ f_3=\begin{cases} 0 \text{ si } 0\le Z_\alpha\le 0{,}01 \\ \frac{0{,}1-Z_\alpha}{0{,}09} \text{ si } 0{,}01\le Z_\alpha\le 0{,}1 \\ 1 \text{ si } 0{,}1\le Z_\alpha\le 1 \end{cases} \\ f_2=\begin{cases} 0 \text{ si } 0\le Z_\alpha\le 0{,}01 \\ 1-\frac{0{,}1-Z_\alpha}{0{,}09} \text{ si } 0{,}01\le Z_\alpha\le 0{,}1 \\ 1 \text{ si } 0{,}1\le Z_\alpha\le 0{,}9 \\ 1-\frac{Z_\alpha-0{,}9}{0{,}09} \text{ si } 0{,}9\le Z_\alpha\le 0{,}99 \\ 0 \text{ si } 0{,}99\le Z_\alpha\le 1 \end{cases} \end{gathered} \tag{14}$$

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

5 Integration of the model

The integration of the model is ensured by the generator of MFront code.

6 Bibliography

1) Helfer T, Castelier E, "LE generator of code will mfront: general presentation and application to the properties material and the models "

On line: http://tfel.sourceforge.net/documents/mfront/mfront.pdf