Models of metallurgical behavior of the zircaloy

Summary :

This document presents the models of metallurgical behavior describing structure transformations, with the heating and with the cooling, which the zircaloy (sheath of fuel pencil) undergoes enters approximately $700\,°C$ and $1000\,°C$.

Contents

1 Introduction

The fuel sheaths of the nuclear reactors with pressurized water consist of zirconium alloy. These alloys undergo metallurgical transformations enters $700\,°C$ and $1000\,°C$, where they pass from a phase of compact hexagonal structure to a phase of cubic structure. In certain cases of analysis the such scenarios of accident of heart per primary education loss of cooling agent (APRP), the sheath reaches temperatures of the order $1000\,°C$ and undergoes metallurgical transformations then. To analyze the mechanical behavior of the sheath in these situations, it is necessary to take into account the influence of the metallurgy on mechanics (modification of the mechanical characteristics).
This document relates to the modeling of structure transformations of Zircaloy to the heating and cooling and this, on a scale which, while remaining “reasonable” for the metallurgist, is easily usable by the mechanic.

Metallurgy calculations in *Code_hasster* are done either during the integration of the mechanical law of behavior, or with the dedicated operator CALC_META, in “post - treatment” of a thermal calculation of evolution. In this second case; LE choice of the model is done with the keyword RELATION = ‘ZIRC’ under BEHAVIOR. This kind of modeling is realizable within *Code_Aster* for the whole of the elements (PLAN, AXIS, 3D) PHENOMENON “THERMICS“. For the definition of the metallurgical behavior of Zircaloy the information of the keyword factor META_ZIRC under the order DEFI_MATERIAU [U4.43.01] is necessary. Lastly, the definition of the initial metallurgical state is realizable using the order CREA_CHAMP, under the keyword factor ETAT_INIT of the operator CALC_META.

Models established in *Code_Aster* to model the metallurgical transformations of Zircaloy are models developed by the ECA. These models were identified on the basis of test of dilatometry and calorimetry for alloys of sheaths (standard and new).

For the mechanical behavior with effect of structure transformations, one has the choice between several models:

- Shears the same relations of mechanical behavior developed initially for the steel of tank 16MND5. They are all the relations declared in the operator STAT_NON_LINE under the keyword BEHAVIOR type META_XX_XX. These are models elastoplastic or elastoviscoplastic, isotropic work hardening (linear or not linear) or kinematics, taken into account or not of the phenomena of plasticity of transformation and restoration of metallurgical work hardening of origin (cf R4.04.02 and R4.04.03).
- Sthe law specific to Zircaloy hears. It is about a model élastovisqueux without threshold and anisotropic (matrix of Hill). The keyword under BEHAVIOR is META_LEMA_ANI (cf R4.04.05) in this case, the metallurgical phase is an internal variable of the law of behavior and is given during the integration of this one.

2 Presentation of the model

2.1 Proportion with balance

Zircaloy has a compact hexagonal structure called phase α, stable until temperatures about $700\,°C$. Beyond approximately $700\,°C$ starts an allotropic transformation towards a cubic phase β, and which is complete around $975\,°C$.
The proportion of the phase Z_β^{eq} to balance is given by the equation, of type Johnson-Mehl-Avrami, following:

$$\begin{cases} Z_\beta^{eq}=0 & \text{pour} \quad T\leq T_d^{eq} \\ Z_\beta^{eq}=1-\exp\left(-\left(K\left(T-T_d^{eq}\right)\right)^n\right) & \text{pour} \quad T_d^{eq}\leq T\leq T_f^{eq} \\ Z_\beta^{eq}=1 & \text{pour} \quad T>T_f^{eq} \end{cases} \tag{1}$$

where T_d^{eq} is the initial temperature of transformation $\alpha\Leftrightarrow\beta$ with balance, T_f^{eq} the temperature of end of transformation to balance, T the temperature and K and n two parameters materials.
In an equivalent way, by reversing the equation 1, the equivalent temperature is obtained T^{eq} according to the proportion Z_β of phase β :

$$\begin{cases} T^{eq}=T_d^{eq}+\dfrac{1}{K}\left(\log\left(\dfrac{1}{1-Z_\beta}\right)\right)^{1/n} & \text{pour } 0\leq Z_\beta\leq 0{,}99 \\ T^{eq}=T_f^{eq} & \text{pour } 0{,}99\leq Z_\beta\leq 1 \end{cases} \tag{2}$$

The temperature of end of transformation to balance T_f^{eq} is selected such as correspondent with a proportion $0{,}99$ of phase β transform, is:

$$T_f^{eq}=T_d^{eq}+\frac{1}{K}\left(\log\left(\frac{1}{1-0{,}99}\right)\right)^{1/n} \tag{3}$$

2.2 Equation of evolution to the heating

The transformation with the heating is the transformation $\alpha\Rightarrow\beta$.
The initial temperature of transformation of phases to the heating T_c depends on the speed of temperature to the heating and is given by the equation:

$$T_c=T_c^1\left(V_{ch}\right)^{T_c^2} \tag{4}$$

With V_{ch} heating rate in $°C/s$ and $T_c\geq T_d^{eq}$.
The model of evolution of the phase β to the heating is given by the differential equation (model of Holt) following:

$$\frac{dZ_\beta}{dt}=A_c\exp\left(-\frac{E}{RT}\right)\left|T-T^{eq}\left(Z_\beta\right)\right|^M \tag{5}$$

$T^{eq}\left(Z_\beta\right)$ is the temperature of balance corresponding to the instantaneous proportion Z_β of phase β and given by the equation 2. T_c^1 , T_c^2 , A_c , $\dfrac{E}{R}$ and M are parameters materials.

2.3 Equation of evolution to cooling

The transformation with cooling is the transformation $\beta\Rightarrow\alpha$.

The initial temperature of transformation of phases to cooling T_r depends on the speed of temperature to cooling and is given by the equation:

$$T_r = T_r^1 + T_r^2 \ln(V_{ref}) \quad (6)$$

With V_{ref} the speed of cooling in $°C/s$ and $T_r \leq T_f^{eq}$.
The model of evolution of the phase β to cooling is given by the following differential equation:

$$\frac{dZ_\beta}{dt} = -|T - T^{eq}| \exp\left(A_r + B_r |T - T^{eq}|\right) Z_\beta (1 - Z_\beta) \text{ for } T_d^{eq} \leq T \leq T_f^{eq} \quad (7)$$

T_r^1 , T_r^2 , A_r and B_r are parameters materials.

2.4 Conditions of use of the metallurgical model for unspecified transients of temperature

2.4.1 Some rules

- During calculations, if the proportion of phase β is higher strict than $0,99$, one rounds with one. For a speed with the heating lower than $0.1 °C/s$, one uses $T_c = T_d^{eq}$.
- If $0 \leq Z_\beta \leq 0,99$, one must observe the following rule:
  - If $T > T^{eq} \Leftrightarrow Z_\beta < Z_\beta^{eq}$, one applies the model to the heating (even if the speed of temperature is negative)
  - If $T < T^{eq} \Leftrightarrow Z_\beta > Z_\beta^{eq}$, one applies the model to cooling (even if the speed of temperature is positive)

2.4.2 Algorithm

One considers an unspecified transient of temperature $T(t)$.

> *Note: to calculate the initial temperatures of transformation to the heating T_c and with cooling T_r , it is necessary to calculate the cooling and heating rates, respectively. To calculate them, one uses the method of the slipping secant (and not instantaneous speed) from where stages 1 and 2 below.*

> *Note: once the temperatures threshold T_c or T_r exceeded and as long as the transformation is not total (with the heating or cooling), one integrates the equations of evolution even if the temperature passes by again by the threshold.*

- **Stage 1** : Research of the moment t_d^{eq} (or t_f^{eq}) corresponding to the initial temperature T_d^{eq} (or of end T_f^{eq} , respectively) of transformation to balance.
  - Case where $Z_\beta = 0$ initially: search for t_d^{eq}
  - Case where $Z_\beta = 1$ initially: search for t_f^{eq}

- **Stage 2** : Research of the moment t_c (or t_r) corresponding to the initial temperature of transformation T_c (or T_r , respectively) by using the method of the slipping secant:
  - Case where $Z_\beta = 0$ initially: research of the moment when the temperature $T(t)$ exceed T_c .
    - If $T(t) > T_d^{eq}$, one increments time, one calculates T_c and the following condition is tested:

$$(C1) : T(t) > T_c = T_c^1 \left(\frac{T(t) - T_d^{eq}}{t - t_d^{eq}} \right)^{T_c^2} \quad (8)$$

If the condition $(C1)$ one is true passes at the stage (3).

- If $T(t) \leq T_d^{eq}$ without one reaching T_c, IL is then necessary to bring up to date t_d^{eq} by starting again stage 1 as from the current moment.

- Case where $Z_\beta = 1$ initially: research of the moment when the temperature $T(t)$ pass by again by T_r.
  - If $T(t) < T_f^{eq}$, one increments time, one calculates T_r and the following condition is tested:

$$(\mathrm{C2}) : T(t) < T_r = T_r^1 + T_r^2 \ln\left(\frac{|T(t) - T_f^{eq}|}{t - t_f^{eq}}\right) \quad (9)$$

    If the condition $(C2)$ one is true passes at the stage (3).
  - If $T(t) \geq T_f^{eq}$ without one reaching T_r, it is then necessary to bring up to date t_f^{eq} by starting again stage 1 as from the current moment.

- **Stage 3** : Once T_c (or T_r reached, one calculates step by step the evolution of the fraction of phase β appearing using the equation of Holt (with the heating) or the equation to cooling following the sign of $(Z - Z_{eq})$ and this as long as fraction of phase β remain lower than $0{,}99$ and higher than zero. and even if one passes by a peak of temperature.
- **Stage 4** : So during stage 3, the fraction of phase β becomes equal to 1 (or 0), one starts again stage 1 as from the current moment.

3 Digital formulation

Knowing at the previous moment the temperature and the proportion of phase β and at the moment running temperature, one seeks to determine the proportion of phase β at the moment running Z_β^t.
At a given moment, one seeks the solution Z_β^t such as $G(Z_\beta^t)=0$, equation which is solved by a method of Newton with controlled terminals:

$$Z_\beta^{i+1}=Z_\beta^i-\frac{G(Z_\beta^i)}{G'(Z_\beta^i)} \tag{10}$$

The criterion of stop is given by the following condition:

$$\text{Si } G(Z_\beta^{i+1})\leq 10^{-6} \text{ alors } Z_\beta^{i+1}=Z_\beta^t \tag{11}$$

3.1 Determination of the direction of the evolution

To know which is the model to be integrated into one moment t given, it is enough to make the following observations:

- If $Z_\beta^{t-1}<Z_\beta^{eq}(T^t)$ and if one integrates the model into cooling, one will have obligatorily $Z_\beta^t<Z_\beta^{t-1}<Z_\beta^{eq}(T^t)$. However, this is contrary in the condition for application of the model to the cooling which supposes that $Z_\beta^t>Z_\beta^{eq}(T^t)$. It is thus necessary to choose the model with the heating.
- If $Z_\beta^{t-1}>Z_\beta^{eq}(T^t)$ and if one integrates the model into the heating, one will have obligatorily $Z_\beta^t>Z_\beta^{t-1}>Z_\beta^{eq}(T^t)$. However, this is contrary in the condition for application of the model to the heating which supposes that $Z_\beta^t<Z_\beta^{eq}(T^t)$. It is thus necessary to choose the model with cooling.

3.2 Integration of the equations

3.2.1 Model for META_LEMA_ANI

In the case of a use of the law of behavior mechanics `META_LEMA_ANI`, the metallurgical phase is an internal variable of the law of behavior. It is thus given during the integration of that-Ci. The solution of these equations is then ensured by the generator of MFront code.

3.3 Models for the other cases

In any other case, integration is carried out manner following:

- **Model with the heating** : the solution is such as $Z_\beta^{t-1}\leq Z_\beta^t<Z_\beta^{eq}(T^t)$. The function $G_c(Z_\beta)$ and its derivative are given by:

$$G_c(Z_\beta)=Z_\beta-Z_\beta^{t-1}-\Delta t\, A_c\exp\left(-\frac{E}{RT}\right)|T-T_{eq}|^M \tag{12}$$

$$G'_c(Z_\beta)=1+M\,\Delta t\, A_c\exp\left(-\frac{E}{RT}\right)|T-T_{eq}|^{M-1}T'_{eq} \tag{13}$$

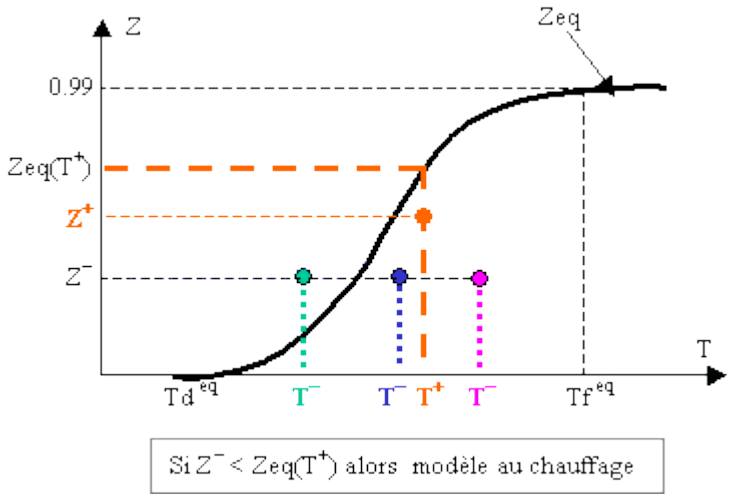
- **Model with cooling** : the solution is such as $Z_\beta^{eq}(T^t)<Z_\beta^t\leq Z_\beta^{t-1}$. The function $G_r(Z_\beta)$ and its derivative are given by:

$$G_r(Z_\beta)=Z_\beta-Z_\beta^{t-1}+\Delta t|T-T_{eq}|\exp\left(A_r+B_r|T-T_{eq}|\right)Z_\beta|1-Z_\beta| \tag{14}$$

$$G'_c(Z_\beta)=1+\Delta t|T-T_{eq}|\exp\left(A_r+B_r|T-T_{eq}|\right)(1-2Z_\beta)$$
$$-\Delta t\, sig(T-T_{eq})T'_{eq}\exp\left(A_r+B_r|T-T_{eq}|\right)Z_\beta(1-Z_\beta)\{1+B_r|T-T_{eq}|\} \quad (15)$$

With:

$$\begin{cases} \text{Si } Z_\beta=0 & \text{pour } T'_{eq}=1000 \\ \text{Si } 0<Z_\beta\leq 0.99 & \text{pour } T'_{eq}=\dfrac{1}{Kn}\left(\log\left(\dfrac{1}{1-Z_\beta}\right)\right)^{\frac{1}{n}-1}\dfrac{1}{1-Z_\beta} \\ \text{Si } 0{,}99<Z_\beta\leq 1 & \text{pour } T'_{eq}=T'_{eq}(0{,}99) \end{cases} \quad (16)$$



4 Model ZIRC in *Code_Aster*

4.1 Internal variables

Internal variables of the relation of behavior 'ZIRC' Shave:

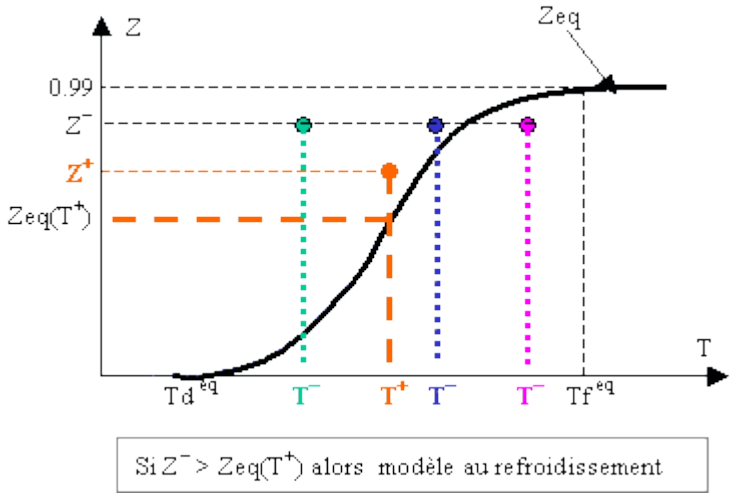
V1 : $Z_{\alpha 1}$ proportion of the phase alpha1,

V2 : $Z_{\alpha 2}$ proportion of the phase alpha2,

V3 : TP, temperature with the nodes,

V4 : t_d^{eq} or t_f^{eq} correspondent with T_d^{eq} or T_f^{eq}, respectively.

The proportion of the phases α and β is given by: $Z_\alpha = Z_{\alpha 1} + Z_{\alpha 2}$ et $Z_\beta = 1 - Z_\alpha$ with the following relations:



Si $0 \le Z_\alpha \le 0.9$ alors $Z_{\alpha 1} = 0, Z_{\alpha 2} = Z_\alpha$ et $Z_\beta = 1 - Z_\alpha$

- Si $0.9 \le Z_\alpha \le 1$ alors $Z_{\alpha 1} = \frac{Z_\alpha - 0.9}{0.1} 0, Z_{\alpha 2} = Z_\alpha - Z_{\alpha 1}$ et $Z_\beta = 1 - Z_\alpha$

In the long term, variables V1 and V2 will disappear to only store Z_α in V1.

Notice : one considers for the parameters materials of the mechanical model, 3 different phases: α, αβ and β, this is why two phases V1 and V2 are stored. However the relations above are not adapted.

In the mechanical model META_LEMA_ANI, the following relations are considered:

- Si $0 \le Z_\alpha \le 0.01$, on prend les données mécaniques de la phase β
- Si $0.01 \le Z_\alpha \le 0.1$, on prend les données mécaniques de la phase β et αβ
- Si $0.1 \le Z_\alpha \le 0.9$, on prend les données mécaniques de la phase αβ
- Si $0.9 \le Z_\alpha \le 0.99$, on prend les données mécaniques de la phase α et αβ
- Si $0.99 \le Z_\alpha \le 1$, on prend les données mécaniques de la phase α

4.2 Use of the model

In the case of a use of the law of behavior mechanics META_LEMA_ANI, the metallurgical phase is an internal variable of the law of behavior. It is thus given during the integration of that-Ci.
For any other law of behavior, the instructions below are to be respected.

To activate this model, it is enough to inform in the order CALC_META, under the keyword BEHAVIOR, the relation 'ZIRC' (COMPORTEMENT=_F (RELATION=' ZIRC')).
The parameters materials are indicated under the keyword factor META_ZIRC of DEFI_MATERIAU.
Lastly, the definition of the initial metallurgical state is realizable using the order CREA_CHAMP, under the keyword factor ETAT_INIT of the operator CALC_META. It is obligatory to inform the internal variables V1, V2 and V4.

Notice : in theory, the metallurgical initial state is $Z_\alpha = 1$, that is to say $Z_\alpha = 0$ and the variable V4 need does not have to be initially indicated. But, so for an unspecified reason, a user wishes to carry out following calculation: $Z_\alpha = 1$ initially for $T_d^{eq} < T(t) < T_c$ then the moment t_d^{eq} by default with zero will be taken if V4 was not obligatorily well informed. This is why, the variable V4 is obligatory and corresponds to the 1er moment of metallurgical calculation (by necessarily equal to zero).

5 Bibliography

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