Models of metallurgical behavior of the Summarized

zircaloy :

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 $1000\,°C$.

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1 Introduction

the sheaths of fuels of the nuclear engines to pressurized water consists 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 cubic structure phase. 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 structural mechanics behavior of the sheath in these situations, it is necessary to take into account the influence of the metallurgy on the mechanics (modification of the mechanical characteristics).
This document relates to the modelization of structure transformations of Zircaloy to the heating and cooling and this, with a scale which, while remaining "reasonable" for the metallurgist, is easily usable by the mechanic.

Metallurgy computations in *Code_Aster* are done with the operator dedicated CALC_META, in "post - processing" of a thermal computation of evolution. The choice of the model is done with the key word RELATION = "ZIRC" under COMP_INCR. This kind of modelization is realizable within *the Code_Aster* for all the elements (PLANE, AXIS, 3D) of the PHENOMENE "THERMAL". For the definition of the metallurgical behavior of Zircaloy the information of the key word factor META_ZIRC under command DEFI_MATERIAU [U4.43.01] is necessary. Lastly, the definition of the initial metallurgical state is realizable using command CREA_CHAMP, under the key word factor ETAT_INIT of operator CALC_META.

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

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

- That is to say the same behavior models mechanics developed initially for the steel of tank 16MND5. They are all the relations declared in operator STAT_NON_LINE under key word COMP_INCR of type META_XX_XX. These are models elastoplastic or elastoviscoplastic, isotropic hardening (linear or not linear) or kinematics, taken into account or not of the phenomena of plasticity of transformation and restoration of metallurgical hardening of origin (cf R4.04.02 and R4.04.03).
- That is to say the model specific to Zircaloy. It is about a model élastovisqueux without threshold and anisotropic (matrix of Hill). The key word under COMP_INCR is META_LEMA_ANI (cf R4.04.05).

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2 Presentation of the model

2.1 Proportion to the equilibrium

Zircaloy about has a compact hexagonal structure called α phase, stable until temperatures $700\,°C$. 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 the equilibrium is given by the equation, of type Johnson-Mehl-Avrami, following:

$$\begin{cases} Z_\beta^{eq} = 0 & \text{pour } T \le T_d^{eq} \\ Z_\beta^{eq} = 1 - \exp\left\{-\left[K(T - T_d^{eq})\right]^n\right\} & \text{pour } T_d^{eq} \le T \le T_f^{eq} \\ Z_\beta^{eq} = 1 & \text{pour } T > T_f^{eq} \end{cases} \qquad \textbf{éq 2.1-1}$$

where T_d^{eq} is the initial temperature of transformation $\alpha \Leftrightarrow \beta$ to the equilibrium, T_f^{eq} the temperature of end of transformation to the equilibrium, T the temperature and K n two materials parameters.

In an equivalent way, by reversing equation 2.1, one obtains the equivalent temperature T^{eq} according to the proportion Z_β of phase β.

$$\begin{cases} T^{eq} = T_d^{eq} + \dfrac{1}{K}\left[\log\left(\dfrac{1}{1 - Z_\beta}\right)\right]^{1/n} & \text{pour } 0 \le Z_\beta \le 0.99 \\ T^{eq} = T_f^{eq} & \text{pour } 0.99 \le Z_\beta \le 1 \end{cases} \qquad \textbf{éq. 2.1-2}$$

the temperature of end of transformation to the equilibrium T_f^{eq} is selected such as corresponding with 0.99 of transformed β phase, that is to say

$$T_f^{eq} = T_d^{eq} + \frac{1}{K}\left[\log\left(\frac{1}{1 - 0.99}\right)\right]^{1/n} \qquad \textbf{éq. 2.1-3}$$

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 Tc to the heating depends on the velocity of temperature to the heating and is given by the equation:

$$Tc = T_1^c \left(V_{ch}\right)^{T_2^c} \text{ avec } V_{ch} = \text{vitesse au chauffage en °C/s et } Tc \ge T_d^{eq} \qquad \textbf{éq. 2.2-1}$$

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- The model of evolution of the phase β to the heating is given by the differential equation (models of Holt) following:

$$\text{Pour } \mathrm{T} > \mathrm{Tc} \geq T_d^{eq} \qquad \frac{\mathrm{dZ}_\beta}{\mathrm{dt}} = A_c \exp\left(-\frac{E}{R\,\mathrm{T}}\right)\left|\mathrm{T}-\mathrm{T}_{\mathrm{eq}}(\mathrm{Z}_\beta)\right|^M \qquad \textbf{éq. 2.2-2}$$

$\mathrm{T}_{\mathrm{eq}}(\mathrm{Z}_\beta)$ is the temperature of equilibrium corresponding to the instantaneous proportion Z_β of phase β and data by equation 2.1-2

T_1^c, T_2^c, A_c, $\frac{E}{R}$ et M is materials parameters.

2.3 Equation of evolution to cooling

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

- The initial temperature of transformation of phases Tr to cooling depends on the velocity of temperature to cooling and is given by the equation:

$$\mathrm{Tr} = T_1^r + T_2^r \ln \mathrm{V}_{\mathrm{ref}} \text{ avec } \mathrm{V}_{\mathrm{ref}} = \text{vitesse de refroidissement en °C/s et } \mathrm{Tr} \leq T_f^{eq} \qquad \textbf{éq. 2.3-1}$$

- The model of evolution of the phase β to cooling is given by the following differential equation:

$$\text{Pour } \mathrm{T} < \mathrm{Tr} \leq T_f^{eq} \quad \frac{\mathrm{dZ}_\beta}{\mathrm{dt}} = -\left|\mathrm{T}-\mathrm{T}_{\mathrm{eq}}\right| \exp\left(A_r + B_r \cdot \left|\mathrm{T}-\mathrm{T}_{\mathrm{eq}}\right|\right) \cdot \mathrm{Z}_\beta \cdot (1-\mathrm{Z}_\beta) \qquad \textbf{éq. 2.3-2}$$

T_1^r, T_2^r, A_r et B_r are materials parameters.

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

2.4.1 Some rules

- At the time as of computations, if the proportion of phase β is higher strict than 0.99, one rounds with one.
- For a velocity with the heating lower than 0.1°C/s, one uses $\mathrm{Tc} = T_d^{eq}$.
- If $0. \leq Z_\beta \leq 0.99$, one must observe the following rule:
  - If $\mathrm{T} > \mathrm{T}_{\mathrm{eq}} \Leftrightarrow \mathrm{Z}_\beta < \mathrm{Z}_\beta^{\mathrm{eq}}$, one applies the model to the heating (even if the velocity of temperature is negative)
  - If $\mathrm{T} < \mathrm{T}_{\mathrm{eq}} \Leftrightarrow \mathrm{Z}_\beta > \mathrm{Z}_\beta^{\mathrm{eq}}$, one the model applies to cooling (even if the velocity of temperature is positive)

2.4.2 Algorithm

One considers an unspecified transient of temperature $\mathrm{T}(\mathrm{t})$.

> *Note: to compute: the initial temperatures of transformation to the heating Tc and cooling Tr, it is necessary to calculate the cooling and heating rates, respectively (éq. 2.2-1 and*

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éq. 2.3-1). To calculate them, the slipping secant method is used (and not instantaneous velocity) from where stages 1 and 2 below.

Note: once the exceeded temperatures Tc threshold Tr or 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:** Search of time t_d^{eq} (or t_f^{eq}) corresponding to the initial temperature T_d^{eq} (or end T_f^{eq}, respectively) of transformation to the equilibrium.
  - Case where $Z_\beta = 0$ initially: search for t_d^{eq}
  - Case where $Z_\beta = 1$ initially: search for t_f^{eq}

- **Stage 2** : Search of time tc (or tr) corresponding to the initial temperature of transformation Tc (or Tr, respectively) by means of slipping secant method:
  - Case where $Z_\beta = 0$ initially: search of time when the temperature $T(t)$ exceeds Tc.
    - If $T(t) > T_d^{eq}$, time is incremented, one calculates Tc and one tests the following condition:

Si $T(t) > Tc = T_1^c \left(\frac{T(t) - T_d^{eq}}{t - t_d^{eq}} \right)^{T_2^c}$, alors on passe à l'étape 3

    - If $T(t) \le T_d^{eq}$ without one reaching Tc, it is then necessary to bring up to date t_d^{eq} by starting again stage 1 from current time.
  - Case where $Z_\beta = 1$ initially: search of the time when the temperature $T(t)$ passes by again by Tr
    - If $T(t) < T_f^{eq}$, one increments time, one calculates Tr and one tests the following condition:

Si $T(t) < Tr = T_1^r + T_2^r \ln \left(\frac{\left| T(t) - T_f^{eq} \right|}{t - t_f^{eq}} \right)$, alors on passe à l'étape 3

    - If $T(t) \ge T_f^{eq}$ without one reaching Tr, it is then necessary to bring up to date t_f^{eq} by starting again stage 1 from current time.

- **Stage 3:** Once Tc (or Tr) reached, one calculates step by step the evolution of the fraction of phase β appearing using the equation of Holt (to the heating) or of the equation to cooling following the sign of $(Z - Z_{eq})$ and this as long as the fraction of phase β remains lower than 0.99 and the higher than 0. 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 from current time.

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3 Numerical formulation

Knowing $(t^-, T^-, Z_\beta^-, t^+, T^+)$, time less, the temperature at time less, the proportion of phase β at time less, time more and the temperature at time more, respectively, one seeks to determine the proportion of phase β at time more Z_β^+.

A a time more given, one seeks the solution Z_β^+ such as $G(Z_\beta^+) = 0$, equation which is solved by a method of Newton with controlled limits.

$$Z_\beta^{i+1} = Z_\beta^i - \frac{G(Z_\beta^i)}{G'(Z_\beta^i)} \quad \textbf{éq. 3-1}$$

the stopping criteria are given by the following condition:

$$\text{Si } G(Z_\beta^{i+1}) \le 10^{-6}, Z_\beta^{i+1} = Z_\beta^+ \quad \textbf{éq. 3-2}$$

3.1 Determination of the meaning of the evolution

to know which is the model to integrate into a given t^+ time, it is enough to make the following observations:

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

3.2 Integration of the equations

- **Models with the heating** : the solution is such as $Z_\beta^- \le Z_\beta^+ < Z_\beta^{eq}(T^+)$. The function $G^c(Z_\beta)$ and its derivative are given by:

$$G^c(Z_\beta) = Z_\beta - Z_\beta^- - \Delta t . A_c \exp\left(-\frac{E}{RT}\right)\left|T - T_{eq}\right|^M \quad \textbf{éq. 3.2-1}$$

$$G'^c(Z_\beta) = 1 + M\Delta t . A_c \exp\left(-\frac{E}{RT}\right)\left|T - T_{eq}\right|^{M-1} . T'_{eq} \quad \textbf{éq. 3.2-2}$$

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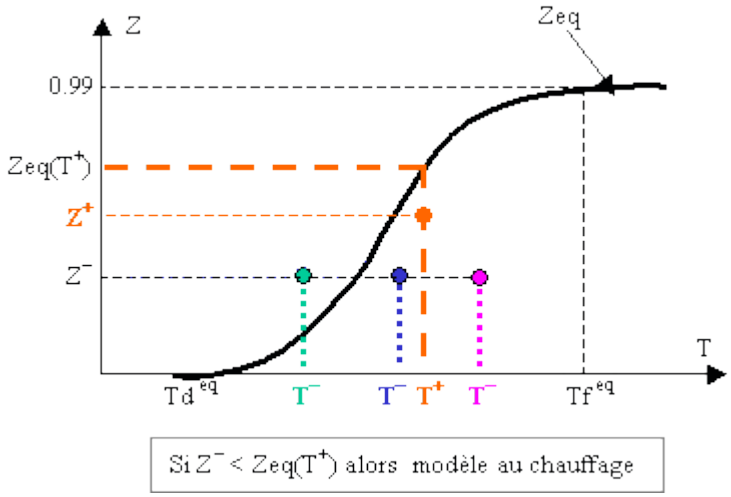
- **Models with cooling** : the solution is such as $Z_\beta^{eq}(T^+) < Z_\beta^+ \le Z_\beta^-$. The function $G^r(Z_\beta)$ and its derivative are given by:

$$G^r(Z_\beta) = Z_\beta - Z_\beta^- + \Delta t.\left|T - T_{eq}\right| \exp\left(A_r + B_r.\left|T - T_{eq}\right|\right).Z_\beta.\left[1 - Z_\beta\right] \qquad \text{éq. 3.2-3}$$

$$G'^r(Z_\beta) = 1 + \Delta t.\left|T - T_{eq}\right| \exp\left(A_r + B_r.\left|T - T_{eq}\right|\right)\left[1 - 2.Z_\beta\right] - \Delta t.sig\left(T - T_{eq}\right)T'_{eq} \exp\left(A_r + B_r.\left|T - T_{eq}\right|\right).Z_\beta \cdot (1 - Z_\beta)\left[1 + B_r\left|T - T_{eq}\right|\right] \qquad \text{éq. 3.2-4}$$

With

$$\begin{cases} \text{Si } Z_\beta = 0, & T'^{eq} = 1000 \\ \text{Si } 0 < Z_\beta \le 0.99, & T'^{eq} = \dfrac{1}{Kn}\left[\log\left(\dfrac{1}{1 - Z_\beta}\right)\right]^{\frac{1}{n}-1} \cdot \dfrac{1}{(1 - Z_\beta)} \\ \text{Si } 0.99 < Z_\beta \le 1, & T'^{eq} = T'^{eq}(0.99) \end{cases} \qquad \text{éq. 3.2-5}$$



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4 Models ZIRC in *Code_Aster*

4.1 Local variables

the local variables of behavior model "ZIRC" are:

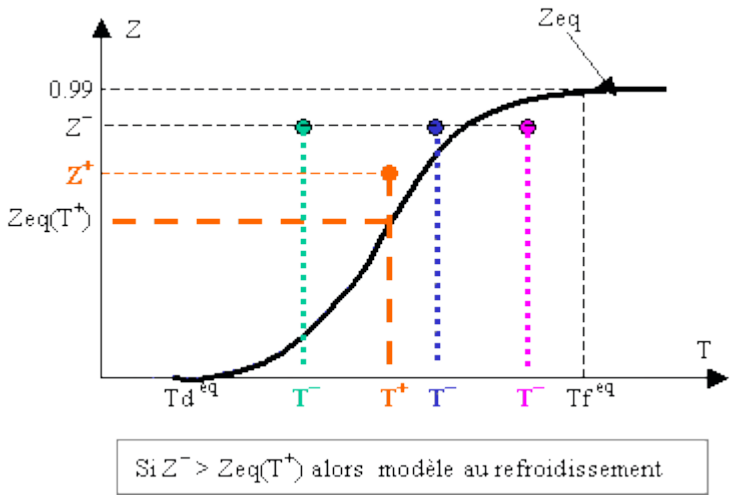
V1: $Z_{\alpha 1}$ proportion of the phase alpha1,

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

V3: TP, temperature with the nodes,

V4: t_d^{eq} or t_f^{eq} corresponding 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 $Z_{\alpha 1} = \dfrac{Z_\alpha - 0.9}{0.1} 0, Z_{\alpha 2} = Z_\alpha - Z_{\alpha 1}$ et $Z_\beta = 1 - Z_\alpha$

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

Note: one considers for materials parameters mechanical model, 3 different phases: α, $\alpha\beta$ and β, this is why two phases V1 and V2 are stored. However the relations above are not adapted.

In the model mechanical 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 $\alpha\beta$
- Si $0.1 \le Z_\alpha \le 0.9$, on prend les données mécaniques de la phase $\alpha\beta$
- Si $0.9 \le Z_\alpha \le 0.99$, on prend les données mécaniques de la phase α et $\alpha\beta$
- Si $0.99 \le Z_\alpha \le 1$, on prend les données mécaniques de la phase α

4.2 Use of the model

to activate this model, it is enough to inform in command CALC_META, under the key word COMP_INCR, relation "ZIRC" (COMP_INCR=_F (RELATION=' ZIRC')).
Materials parameters are well informed under factor key word the META_ZIRC of DEFI_MATERIAU.

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Lastly, the definition of the initial metallurgical state is realizable using command CREA_CHAMP, under the key word factor ETAT_INIT of operator CALC_META. It is compulsory to inform the local variables V1, V2 and V4.

Note: in theory, the metallurgical initial state is either $Z_\alpha = 1$, or $Z_\alpha = 0$ and the variable V4 does not need to be initially indicated. But, so for an unspecified reason, an user wishes to carry out following computation: $Z_\alpha = 1$ initially for $T_d^{eq} < T(t) < T_c$ then time t_d^{eq} by default with zero will be taken if V4 were not obligatorily indicated. This is why, the variable V4 is compulsory and corresponds to the 1st metallurgical time of computation (by necessarily equal to zero).

5 Bibliography

1) Blacksmith, T., and al., “Experiment and modeling of advanced fuel rod cladding behavior under LOCA conditions: A-B phase transformation kinetics and EDGAR methodology”, Zirconium in the Nuclear Industry: International Twelth Symposium, 1998, Toronto, ASTM STP 1354, Historical

6 ASTM of the versions of the document

Version Aster	Author (S) or contributor (S), organization	Description of the modifications
5	A.RAZAKANAIVO	initial Text
9.4	V.CANO	Modifications of the model concerning the initial temperatures of transformation, which depend on the velocity of transformation, and new method of resolution

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