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Kommentar

Strålsäkerhetsmyndigheten
Att: Ansi Gerhardsson
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Svar till SSM på begäran om förtydligande angående krypmodell för OFP-koppar och implementering av modellen i ABAQUS

Strålsäkerhetsmyndigheten, SSM, har i skrivelse till Svensk Kärnbränslehantering AB, SKB, begärt förtydligande av ansökan om slutförvaring av använt kärnbränsle och kärnavfall angående krypmodell för OFP-koppar och implementering av modellen i ABAQUS. SSM:s frågor är uppdelade i två bilagor vilka även detta svarsbrev speglar. SSM:s frågor återges nedan i kursiv text och besvaras punkt för punkt. Frågorna är ställda på engelska och besvaras därför också på engelska.

Med vänlig hälsning

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Bilaga 1

Questions to SKB regarding the creep model used in SKB's FE analyses of the copper canister

Questions below are related to the creep model described in reference [1].

[1] Rolf Sandström and Henrik C.M. Andersson, Creep in phosphorus alloyed copper during power-law breakdown, J. Nuc. Mat., 372 (2008) 76-88. (same as "Sandström and Andersson (2008a)")

General

In the paper by Sandström and Andersson (2008a) several creep models are presented. The answers below primarily refer to the creep model used by Hernelind in FEM calculations for SKB on the copper canister. The model is specified in SKBdoc 1482373. The creep model is also described in the publications by Sandström and Andersson (2008b), Jin and Sandström (2009) and Raiko et al. (2010). In the text below the original questions from SSM are given in italics and SKB's answers in normal text. The equation numbers in both the questions and the answers refer to Sandström and Andersson (2008a).

QUESTIONS

1. *How should g_{rate} be understood? Is it a scale factor dependent only on temperature that relates initial creep strain rate with the minimum creep strain rate?*

The models for primary creep in Sandström and Andersson (2008a) are based on the so called μ model (Wu et al. 2004) that gives an exponential dependence for both the time and strain dependence of the primary creep rate. One form of the μ model has been known since the 1930s and has been extensively used in FEM-based creep calculations in industry. When the precision in the creep testing was improved in the 1990ties, it was demonstrated that the μ model could describe the time and strain dependence of the creep rate in the primary stage to the accuracy of the experiments for martensitic steels, stainless steels and copper. Later it has been shown that it is consistent with a basic model for primary creep of copper (Sandström 2012).

The initial creep rate during primary creep is much larger than during the secondary stationary stage. The ratio between these two creep rates is expressed as g_{rate}. The expression for g_{rate} is derived from the μ model.

$$g_{\text{rate}} = \left(\frac{t_{\text{min}}}{t_{\text{init}}}\right)^{\phi_2/(1+\phi_2)}$$

Since the time to the minimum creep rate t_{min} is related to the rupture time ($t_R/3$) in the model, it depends on both temperature and stress, and as a consequence so does g_{rate}.

In the expression for g_{rate} there are three parameters ϕ_2, t_{init} and t_{min} and in the expression for ω, equation (12), there are three more parameters B, n_b, and p_b. The values of t_{init} = 1 h and $t_{min} = t_R/3$ have been selected to make a comparison to experiments easy to handle. The remaining four parameters ϕ_2, B, n_b, and p_b have then been fitted to experimental creep curves and slow strain stress curves.

2. *What is the value of N in equation (14), i.e.* $g_{\text{rate}} = (\frac{\sigma_1}{\sigma_1 - \sigma_{i1}})^N$ *? Is N given by equation (9).*

N is the Norton (creep) exponent. It is given by

$$N = \left.\frac{\partial \log \dot{\varepsilon}_{\text{cr}}}{\partial \log \sigma}\right|_{\text{min}}$$

The final form of *N* depends on the creep model. See also the answer to question 6.

3. *Does determination of* g_{rate} *based on equations (13)/(14) or (29)/(30) give the same* g_{rate}*?*

Equations (13)/(14) are more general than (29)/(30) and can be used for different models. It is recommended to use the expression derived directly from the μ model (eqs. (29) and (30)).

$$g_{\text{rate}} = (\frac{t_{\text{min}}}{t_{\text{init}}})^{\phi_2/(1+\phi_2)}$$

4. *In the application of the creep model in SKB's FE analyses of the copper canister, technological stress is used. In the ABAQUS user subroutine, true stress is reduced according to* $\sigma = \sigma_{true} e^{-\varepsilon^{cr}_{eff}}$ *. Should σ in equation (22) and (43) be technological stress? If yes, how is this explained?*

σ in equations (22) and (43) is a stress that is a correction to the true stress due to stage IV work hardening. In the uniaxial case it happens to be equal to the technological stress. Stage IV work hardening in copper has a very large effect both on stress strain curves and creep curves. It gives a linear stress (true stress) dependence as a function of strain. This is illustrated in Figs. 4 and 7 in Sandström and Andersson (2008a). Since the consequence of stage IV work hardening is exactly the same as if you replace true stresses with engineering stress in the uniaxial case, they were called engineering stresses in Sandström and Andersson (2008a). In retrospective this was unfortunate, because it gave the impression that FEM computations should be made with engineering stresses. However, the factor $e^{-\varepsilon^{cr}_{eff}}$ is vital to take stage IV work hardening into account. The effect of stage IV work hardening was analysed in detail in Sandström and Hallgren (2012).

5. Does the following equation hold for creep in Cu-OFP:

$\Delta\varepsilon_{tot}^{cr} = (\dot{\varepsilon}_{stationary}^{cr} + \dot{\varepsilon}_{non-stationary}^{cr})\Delta t$ *where* $\dot{\varepsilon}_{stationary}^{cr}$ *is given by equation (22) and* $\dot{\varepsilon}_{non-stationary}^{cr}$ *is given by equation (43).*

The answer is model dependent. In the model that Hernelind has used, the non-stationary solution does not automatically include the stationary one and then the two parts should be added. On the other hand, in the primary creep model presented more recently (Sandström 2012), the non-stationary solution already includes the stationary part, and then the non-stationary part gives the complete solution.

6. Is the expression in (23), i.e $N = 3 + \frac{2Q_{eff}}{RT}\left(\frac{\sigma}{\sigma_{i\max}}\right)^2$ *correctly derived based on equation (9) and (20)*

The general expression for the Norton exponent is the one given above

$$N = \left.\frac{\partial \log \dot{\varepsilon}_{cr}}{\partial \log \sigma}\right|_{min}$$

If the expression is applied to equation (20) or (22) it gives

$$N = 3 + \frac{2Q_{eff}}{RT}\left(\frac{\sigma}{\sigma_{i\max}}\right)^2$$

The contribution from the factor $\exp(\sigma b^3/k_B T)$ in eqs. (20) and (22) is neglected since it is small. If the Norton exponent is evaluated in the model in equation (7), it gives the result in equation (9).

Bilaga 2

Questions to SKB regarding the implementation of the creep model into ABAQUS

Questions below are related to the implementation of the creep model described in reference [1] into ABAQUS.

[1] Rolf Sandström and Henrik C.M. Andersson, Creep in phosphorus alloyed copper during power-law breakdown, J. Nuc. Mat., 372 (2008) 76-88. (same as "Sandström and Andersson (2008a)")

General

Creep simulations in copper have been performed for the copper shell of the KBS-3 canister in the final repository of spent nuclear fuel. The FE-code ABAQUS (ABAQUS 2014) has been used for the simulations and when including creep in the simulation a user defined subroutine has been used.

The subroutine is based on the theory for phosphorus alloyed copper presented by Sandström and Andersson (2008a) and a report (SKBdoc 1482373) describing how the routine shall be used.

There exist a lot of predefined subroutine interfaces which could be used for ABAQUS (ABAQUS 2014), and for creep two possibilities are available, subroutine interface CREEP and the subroutine interface UMAT. The CREEP interface is the easiest way to implement traditional creep theory and assumes that the magnitude of the creep strain is driven by Mises effective stress. This method is used to implement the creep material model used for the simulations involving creep in copper (SKBdoc 1482373).

QUESTIONS

1. It is unclear how g_{rate} is derived in the user subroutine. Can this be further explained?

$g_{\text{rate}} = (\frac{t_{\text{min}}}{t_{\text{init}}})^{\phi_2/(1+\phi_2)}$ is calculated based on Andersson-Östling and Sandström, (2007) using Equations (19) and (22) together with the text defining t_{min} and t_{init}. The time ratio g_{rate} in Eq. (22) can be estimated by assuming that $t_{\text{init}} \sim 1$ h and $t_{\text{min}} \sim t_R/3$ where t_R is the rupture time. It is evident from Fig. 5b that the creep strain in the primary stage does not vary dramatically with time and hence the exact choice of the parameters t_{init} and t_{min} is not critical.

2. In the user subroutine, the technological stresses $\sigma = \sigma_{true} e^{-\varepsilon_{eff}^{cr}}$ is used in equation (22) and $\sigma_{eff} = (\sigma_{true} - \sigma_i) e^{-\varepsilon_{eff}^{cr}}$ is used in equation (43). What motivates the use of technological stress? How is the factor $e^{-\varepsilon_{eff}^{cr}}$ derived?

The question about technological stresses has been answered above in question 4 to appendix (Bilaga) 1.

The factor $e^{-\varepsilon_{eff}^{cr}}$ is calculated based on $\sigma_{true} = \sigma_{nom} \cdot ln\left(\frac{l}{l_0}\right)$. ABAQUS is using logarithmic strain $\varepsilon = ln\left(\frac{l}{l_0}\right) => n\left(\frac{l}{l_0}\right) = e^{\varepsilon}$. Thus $\sigma_{nom} = \sigma_{true} \cdot e^{\varepsilon}$. Since elastic strains are small, the effective creep strain can be used in this expression.

3. According to equation (35) in [1], the Mises stress $J(\boldsymbol{\sigma} - \boldsymbol{\sigma}_i)$ shall be derived based on the stress tensor and the back stress tensor. In the user subroutine, $J(\boldsymbol{\sigma} - \boldsymbol{\sigma}_i)$ is instead derived as $\sigma_{Mises} - \sigma_i$. Thus, is not considered when calculating the Mises stress. How is this deviation from the creep model motivated? What impact does the deviation have on the numerical results?

Using the CREEP interface, the creep is defined by scalars (no tensors are available). For multi-axial usage this is handled directly by ABAQUS which calculates the strain components using the equivalent (uniaxial) deviatoric creep increment returned from CREEP and using the deviatoric stress gradient.

$$\Delta\boldsymbol{\varepsilon}^{creep} = \frac{1}{3}\Delta\bar{\varepsilon}^{swelling}\boldsymbol{R} + \Delta\bar{\varepsilon}^{creep}\boldsymbol{n}$$

So, by using CREEP, it's not possible to use tensors. However, for the applications where the creep material model have been used, the loading mostly is monotonic which means that the difference should be small (using tensor formulation makes it possible to simulate the Bauschinger effect which occur at cyclic loading). SKB considers this simplification to be reasonable. A comparison between a scalar and tensor formulation has not been performed.

4. For the multiaxial case in [1], the evolution of the back stress tensor $\boldsymbol{\sigma}_i$ is given by equation (39), i.e. $\frac{d\boldsymbol{\sigma}_i}{d\varepsilon_{eff}^p} = \frac{2}{3}\, a_k \frac{d\boldsymbol{\varepsilon}^p}{d\varepsilon_{eff}^p} - c_k\boldsymbol{\sigma}_i$. In the user subroutine, the evolution of the back stress is instead given by the scalar equation (5), i.e. $\frac{d\sigma_i}{d\varepsilon} = \omega(C - \sigma_i)$. How is this deviation from the creep model motivated? What impact does the deviation have on the numerical results?

The subroutine CREEP is based on **USE OF EFFECTIVE STRESS** and is thus not following **MULTIAXIAL FORMULATION.** Bold expressions refer to the headlines in Sandström and Andersson (2008b). SKB considers also this simplification to be reasonable. A comparison between a scalar and tensor formulation has not been performed.

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Jin L Z, Sandström R, 2009. Non-stationary creep simulation with a modified Armstrong–Frederick relation applied to copper canisters. Computational Materials Science 46, 339–346.

Raiko H, Sandström R, Rydén H, Johansson M, 2010. Design analysis report for the canister. SKB TR-10-28, Svensk Kärnbränslehantering AB.

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Sandström R, Hallgren J, 2012. The role of creep in stress strain curves for copper. Journal of Nuclear Materials 422, 51–57.

Wu R, Sandström R, Seitisleam F, 2004. Influence of extra coarse grains on the creep properties of 9 percent CrMoV (P91) steel weldment. Journal of Engineering Materials and Technology 126, 87–94.

Unpublished documents

SKBdoc id, version	Title	Issuer, year
1482373 ver 1.0	Documentation of subroutine for copper creep.	SKB, 2015