Application of a physically-based dislocation creep model to P92 for constructing TTR diagrams

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ABSTRACT
To raise the efficiency of thermal power plants, operation temperature and pressure must be increased by improving the creep performance of materials such as martensitic Cr-steels. To understand the underlying mechanisms of degradation, physical creep modelling provides a detailed and profound insight into microstructural processes. For such a physically based dislocation creep model, it is demonstrated that based on a parameter set found for one experimental creep curve, numerous creep curves on different stress levels can be simulated without any additional experimental data. These simulation results are then used for constructing a TTR diagram of P92. We succeeded in extrapolating rupture times for variations in both applied stress and temperature. In all cases, microstructural evolution of the simulated material is considered, including dislocation density, subgrain size and precipitates. The obtained rupture times in the simulated TTR diagram are compared to reference data, achieving good agreement.

INTRODUCTION
Thermal power plants contain components made out of creep-resistant materials, which are able to withstand high temperatures and mechanical stresses in the range of typically 300 MPa/500°C–50 MPa/650°C [1]. To fulfill these demands, martensitic Cr-steels are predestined. One candidate, the steel X10CrWMoVNb 9–2 (better known as P92), will later be discussed in more detail. To predict the lifetime of relevant components, such as heat exchangers, boilers, pipes e.g.- and to avoid unacceptable deformation or even accidental failures, creep experiments are needed. Unfortunately, creep experiments are very time-consuming and costly. This motivates both industry and science to partly replace experiments by simulation, which is faster and cheaper. However, to describe the phenomenon of creep purely on basis of mathematical, analytical functions is risky, since such phenomenological models lack a deeper physical understanding and may easily lead to overestimated lifetimes. Therefore, physical models have been developed, aiming at linking the microstructure and its evident changes to macroscopic properties. In the frame of this work, we want to introduce a model of this second category and present its potentials and opportunities for calculating creep curves and TTR diagrams of P92.

APPLIED CREEP MODEL
P92 steel consists of martensitic blocks, packets and laths which are located inside prior austenitic grains (PAG). During N + T heat-treatment, also formation of low-angle1 subgrain boundaries and precipitation of secondary phases (carbides, nitrides or intermetallic phases) are observed. Moreover, numerous dislocations – of different type and in various configurations – are spread throughout the microstructure.

In the course of creep exposure, temperature-, stress- and time-dependent evolution of most named microstructural elements (which also affect each other) starts to occur. The most famous relationship in this context is known as Orowan’s law [2], linking the creep strain rate, \( \dot{\epsilon} \), directly to glide velocity and the density of mobile dislocations, \( \rho_m \). However, instead of a glide velocity as in the original formulation, we use here an effective velocity, \( v_{\text{eff}} \), attributed to dislocations interacting with particles inside subgrains, when surmounting them by climb [3,4] (see Equation (1) as well as reaction (9) in Figure 1). \( b \) stands for Burgers vector and \( M \) for Taylor factor.

\[
\dot{\epsilon} = \frac{b}{M} \cdot \rho_m \cdot v_{\text{eff}}
\]

Apart from mobile dislocations \( \rho_m \) and boundary dislocations \( \rho_b \) related to subgrain radius \( R_{\text{sub}} \), static dislocations \( \rho_s \) and precipitates have to be...
considered [5], when setting up a physical dislocation creep model [4] for P92 or similar martensitic steels. These microstructural constituents lead to a framework of four differential rate equations \((\dot{\rho}_m, \dot{\rho}_n, \dot{\rho}_b, \dot{R}_{\text{gb}})\), each taking into account production, annihilation and interaction processes to happen. For an overview of how \(\rho_m, \rho_n, \rho_b, R_{\text{gb}}\) and precipitates (with number density \(N_{\text{V,ij}}\) and radius \(r_i\)) are linked, see Figure 1. The following reactions are included in the model [4]:

To sufficiently model precipitate nucleation, growth and coarsening based on the SFFK theory [7], a separate thermokinetic calculation is carried out in software MatCalc, before importing the result \((r_i, N_{\text{V,ij}})\) into the creep equation framework and thus coupling the two simulations.

For the chemistry of P92 in the simulation, ASTM A335 mean values (e.g. stated in [8]) were adopted, see Table 1:

As virtual heat treatment, 30 min of normalising at 1050°C and 1 h of tempering at 765°C were implemented.

The particles simulated in MatCalc are Laves phase, MX carbo-nitrides (which were split into VN and NbC), \(\text{M}_{23}\text{C}_6\), AlN and modified Z-phase CrVN. Selected nucleation sites were grain boundaries (for VN, NbC), subgrain boundaries (for VN, NbC, Laves, \(\text{M}_{23}\text{C}_6\)) and dislocations (for VN, NbC, AlN) as well as VN on-particle nucleation for Z-phase [9] (to reflect the phenomenon that it gradually transforms from VN). The simulation result of P92 aged for 100,000 hours at 650°C (923 K) – after preliminary normalising and tempering can be seen in Figure 2 (mean diameters) and Figure 3 (number densities). This thermokinetic simulation result is stated here because it represents an important input for the creep simulation.

\(\text{M}_{23}\text{C}_6\), Laves and VN turn out to have the highest molar phase fractions \((\text{M}_{23}\text{C}_6 \approx 2\%, \text{Laves} = 1\%, \text{VN} = 0.5\%)\). Whereas Laves and \(\text{M}_{23}\text{C}_6\) coarsen drastically, VN behaves much more stable in the course of long-term ageing. Z-phase (although huge in size right from the beginning) only starts to play a role after several 10,000 h of ageing, when its molar phase fraction reaches a certain critical amount.

The last missing part in the mosaic of creep is the impact of damage, which becomes important in the tertiary regime of creep. In that way, a hybrid creep model can be created [10] by combining dislocation creep [5] with continuum damage [11]. Two damage parameters are added to Orowan’s law (see Equation (2)): \(D_{\text{cav}}\) for cavitation damage [10] and \(D_{\text{ppt}}\) for precipitate damage as calculated in [4].

### Table 1. P92 chemistry for the thermokinetic simulation in MatCalc.

| Element | Fe   | Al  | C   | Cr  | Mn  | Mo  | N   | Nb  | Ni  | Si  | V   | W   |
|---------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Bal     | 0.01 | 0.10| 9.0 | 0.45| 0.45| 0.05| 0.064| 0.35| 0.35| 0.20| 1.75| [wt.%] |

![Figure 1.](image1.png)

Figure 1. Microstructural constituents and their reactions in the creep model [6].

![Figure 2.](image2.png)

Figure 2. Simulated mean diameter of P92 for 650°C ageing.
Model setup

Step 1:
To calculate a master creep curve for one reference temperature and stress (e.g. 650°C and 118 MPa), the following input parameters have to be defined [4]:

1. Microstructural start values of the material’s as-received state (before creep) are needed as start conditions for solving the four rate equations; they may stem from experiment or literature.
2. Precipitate data come from the preliminary MatCalc simulation and are loaded time-dependent/step-wise into the creep code (for Zener drag, \(v_{\text{eff}}\) and damage).
3. The activation volume for dislocation glide, \(V_r\) (expressed as multiple of the atomic volume, \(\Omega\)) is determined from experimental relaxation data [12] and calculated according to [13]. It turns out that relaxation data slightly overestimate \(V_r\) within creep experiments (see [4]). We thus corrected \(V_r\) accordingly.
4. Four fit-parameters (three of them physical) have to found by using one experimental creep curve
   - Glide velocity pre-factor (\(a_1\)); not accessible by measurements.
   - Density of sources for mobile dislocations (\(\beta\)); not accessible either.
   - Holt constant for subgrain nucleation (\(K_c\)); only available for pure metals [14].
   - Cavitation damage pre-factor \(A\); entirely phenomenological.
5. 16 further physical parameters and 2 fundamental constants; from literature, see details [4]

\[
\dot{\varepsilon}_D = \frac{\dot{\varepsilon}}{(1 - D_{\text{cav}}) \cdot (1 - D_{\text{ppt}})}
\]
For an overview of the most important input parameters for the creep model, see Table 2.

Step 2: For extrapolation with respect to applied stress at 650°C, all above-stated parameters are kept constant and remain completely unchanged. Out of the calculated set of creep curves and the corresponding rupture times, a TTR diagram can be deduced.

Step 3: For extrapolation with respect to temperature from 650°C to 600°C, 3 types of input parameters have to be adapted:

- Precipitate data (new MatCalc simulation at 600°C); slower coarsening rate
- Diffusion speed (lattice diffusion coefficient $D_v$)
- Activation volume $V_a$ (because of different relaxation behaviour at 600°C)

An overview of changes for the temperature extrapolation are shown in Table 3. $\rho_d$ stands for the coarsening constants of VN and $M_{23}C_6$, which represent the changes in MatCalc, comparing 650°C and 600°C ageing for $10^5$ h.

### Table 2. Parameter settings for the creep simulation at 650°C.

| Param. | Value | Source | Param. | Value | Source |
|--------|-------|--------|--------|-------|--------|
| $\rho_{d,0}$ | 6.2 - 10$^{-14}$ m$^{-2}$ | [18,20] | $a_1$ | 5.55 m/s | Fit |
| $\rho_{d}$ | 6.2 - 10$^{-13}$ m$^{-2}$ | 0.1 - $\rho_{d,0}$ [11] | $A$ | 325 | Fit |
| $\rho_{h,0}$ | 5.9 - 10$^{-14}$ m$^{-2}$ | [15] | $\beta$ | 0.0375 | Fit |
| $R_{sph,0}$ | 0.4 µm | [15] | $K_i$ | 2 | Fit |
| $V_i$ | 25Ω | [12,13] |        |       |        |

### Table 3. Parameter changes for creep simulation at 650°C vs. at 600°C.

| Param. | 650°C Setting | Source | 600°C Setting | Source |
|--------|---------------|--------|---------------|--------|
| $V_i$ | 25Ω | [12,13] | 16Ω | [13,16] |
| $D_v$ | 2 - 10$^{-29}$ m$^{-2}$/s | [17] | 2 - 10$^{-30}$ m$^{-2}$/s | [17] |
| $k_{M_{23}C_6}$ | 2.9 - 10$^{-29}$ m$^{-2}$/s | MatCalc | 1.1 - 10$^{-29}$ m$^{-2}$/s | MatCalc |
| $k_{VN}$ | 2.1 - 10$^{-33}$ m$^{-2}$/s | MatCalc | 9.2 - 10$^{-33}$ m$^{-2}$/s | MatCalc |

**Results**

Step 1: Figure 4 shows the result of the simulated master creep curve compared to a measured creep curve (adopted with permission from [18]) for an applied stress of 118 MPa at 650°C, obtaining excellent agreement and achieving a nearly identical creep curve shape. Primary creep zone is fully developed, secondary creep has the same slope and tertiary creep regime is sufficiently well modelled. 100 % damage, respectively, rupture in the simulation occur after 7.8 % of strain or 1135 hours. In the measurement, rupture happened after 1271 hours [18]. This means a simulation inaccuracy of only 10 % with respect to rupture time, entitling any strain above 8 % to be neglected when modelling creep rupture of P92 for the selected conditions.

Important microstructural changes during modelled creep of P92 are illustrated in Table 4, comparing as-received stage (creep start) and 1135 h creep at 118 MPa, 650°C (creep end).

Step 2: The results of all calculated creep curves for varying applied stresses at 650°C are depicted in Figure 5. The stress was varied between 60 and 150 MPa in 10 MPa steps. Agreement with reference data from ECCC is very good for ≤110 MPa. Above 120 MPa, an underestimation of lifetime (up to 30 %) in the simulation can be seen.

Step 3: With the rupture times of all modelled creep curves, it is possible to deduce a TTR diagram, as can be seen in Figure 6. Finally, an extrapolation with respect to temperature (from 650°C to 600°C) is carried out. The result was also added to Figure 6 and compared with ECCC reference data [19]. Between stresses from 120 MPa to 180 MPa, all modelled rupture times at 600°C – calculated in 10 MPa steps – show excellent agreement with reference data [19].

**Figure 5.** Simulated creep curves of P92 at 650°C between 60 and 150 MPa.
with 650°C (chosen stages 1-8). Simulated time-to-rupture (TTR) for P92 steel at 600°C was 1271 h@118 MPa/650°C and 1426 h@140 MPa/650°C.

All three steps in Figure 6 are numbered to point out again how the TTR was constructed: (1) master creep curve calculation/starting point for extrapolation (grey circle), (2) stress extrapolation and (3) temperature extrapolation.

Discussion

Simulated and measured creep curve at 118 MPa/650°C show excellent agreement over all three creep stages (primary, secondary and tertiary regime). Virtual and real sample life is significantly close with 1135 h modelled and 1271 h measured [18]. The obvious discrepancy of 10% with respect to the rupture time is related to interruption of the creep simulation after 8% of strain [18]. After around 8% (chosen as end of simulation), severe necking starts to occur and multiplies the complexity of stress states, which is not included in our model in the current stage.

The agreement of modelled rupture times at 650°C with reference data from ECC [19] is very good in the TTR diagram for σ < 110 MPa and good for σ > 110 MPa, slightly underestimating the reality at higher stresses. At 600°C, all calculated rupture times for σ = 120 MPa to 180 MPa fit perfectly to experimental data in the TTR.

ρm in the simulated master creep curve recovers from 4.5 · 10^{14} m^{-2} in as-received condition to 1.2 · 10^{14} m^{-2} after end of virtual creep at 1135 h. This agrees well to TEM data of ρm = 1 · 10^{14} m^{-2} for P92 steel [20] (1271 h@118 MPa/650°C) and ρm = 1 · 10^{14} m^{-2} for a 10% Cr-steel [21] (1426 h@140 MPa/650°C).

ρb increases from 5.9 · 10^{14} m^{-2} to 7.7 · 10^{14} m^{-2} after end of creep. This behaviour mainly reflects a high number of statics transforming into boundaries [10] (mechanism 3 in Figure 1).

Subgrains coarsen from R_{sub,0} = 0.4 μm in as-received state to R_{sub} = 0.54 μm after end of creep life. A good overview on possible levels of subgrain coarsening in 9–12% Cr-steels is given in [22]. In most observed cases, the values of the subgrain diameters lie between 0.4 and 2 μm [22], which is in line with our simulation. The speed of subgrain coarsening in our model depends on many factors: (a) the Zener pinning effect (see mechanism 7 in Figure 1) and the effectiveness of MX particles to demobilise the subgrains, (b) the nucleation of new subgrains (controlled by the Holt constant) and (c) the role of pipe diffusion affecting the subgrain growth pressure.

Conclusion

Our developed dislocation creep model [4] is capable of physically simulating P92 creep curves with very realistic shape in all three stages of creep. Based on measured strain data from one instrumented creep test, a handful of inaccessible, non-measurable physical parameters are estimated, and a master creep curve is simulated. This was successfully shown here for P92 at 650°C and 118 MPa. After that, extrapolation with respect to stress can be carried out: Out of a calculated series of different
creep curves at 650°C, a TTR diagram has been deduced, showing very good agreement with experimental reference data. For this stress extrapolation, all input parameters remain constant, except for the varying applied stress. A TTR diagram for 600°C has also been constructed. For this temperature extrapolation, precipitate data, activation volume for glide and diffusion coefficients have to be adjusted to the lower temperature level. From this point onward, all input parameters at 600°C remain unchanged, except for the applied stress. Agreement with experimental reference data from ECCC [19] is excellent. Every single point in the deduced TTR framework from the creep simulation is accompanied by a creep curve and defined by a specific time-, stress- and temperature-dependent microstructural status. Subsequently, the evolution of precipitates, dislocations and subgrains is not only the result of an involved differential equation system but it can be demonstrated that the modelled changes on macro- and nano-scale are responsible for the material’s creep response, creep curve shape and high-temperature lifetime.

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Disclosure statement

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