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Mathematical Modeling Applying ν Concept and θ Projection to Creep of Ti-6Al-4V Alloy

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The current materials research field demands sophisticated tests and simulations to predict creep behavior, meet design needs, and save time and resources. This demands an appropriate mathematical formalism that can represent creep data for different materials and loading conditions. In this context, mathematical models such as θ-Projection and ν Concept can be applied to predict the behavior of materials under creep conditions. The main goal of this study involves the application of such methodologies to predict a creep curve for Ti-6Al-4V. In a preliminary assessment, both equation parameters, determined by computational techniques and an experimental database, enabled the determination of the strain-time curve of Ti-6Al-4V at 465 MPa and 500 ºC. The analysis showed that both methods have acceptable accuracy to predict primary, secondary, and tertiary creep behavior for Ti-6Al-4V. However, results indicated that the ν Concept produced a creep curve with better agreement with the experimental data. The technique used for obtaining parameters is promising and should be improved for future research.

Keywords: *Creep, Ti-6Al-4V, Mechanical behavior, Materials characterization, Mathematical modeling.*

1. Introduction

Titanium and its alloys are widely explored in the manufacturing industry in a variety of products for aerospace and automotive applications[1]. In this context, properties such as creep, fatigue, and degradation resistance during service at high temperatures are imperative[2]. Thus, the development of materials able to maintain their structural properties under severe environments and conditions for long periods is an industrial necessity since creep failures are considered the major challenge of this segment[3,4]. Laboratory creep characterization tests often demand investments and a long time to obtain reliable and reproducible results. In this sense, mathematical and simulation models to predict the creep life of materials become allies in the development of aerospace technologies and projects. Furthermore, this assessment method provides great product reliability, decreases project costs, minimizes study time, and dispenses with the use of specimens and complementary characterization tests. As observed, this study field is highly promising, being able to disseminate national technology and create advances in the aerospace industry. These studies involve the elaboration of constitutive equations with the aim to simulate or predict the creep behavior under different stress-temperature regimes.

Therefore, in this study, a critical analysis is carried out based on the constitutive equations called θ-Projection[5] and υ Concept[3,6].

The θ-Projection method is based on an equation that considers the combination of decelerating primary and accelerating tertiary creep stages, enabling its prediction by the interpolation and extrapolation of experimental data[7-9]. The θ-Projection method and its modifications have been applied to predict creep curves for 16MND5 steel (used in reactor pressure vessels)[10], K465 and DZ125 superalloys[11], γ-Titanium Aluminide Ti-45Al-2Mn-2Nb[12], alloy 690 (a material used in steam generator tubes)[13], among others, in which the assessment of the service safety of structural materials were predicted with high agreement. The ν Concept is a mathematical model to express strain-time relations based on the Continuum Damage Mechanics proposed by Barboza[3] and Barboza et al.[6] and inspired by Ion et al.[14] and Kachanov–Rabotnov formalism[15,16]. Creep stages are characterized by the νi operational parameters (i = 1-4) extracted from experimental curves. A preliminary study conducted on Ti–6Al–4V showed great agreement with experimental curves at different stress values at 500-600 °C for short-term tests[3,6]. The main goal of this study involved predicting a creep curve for the Ti-6Al-4V alloy at 465 MPa and 500 °C, using a database generated by determining θ and ν values from six experimental creep curves at different applied stress values. The interpolation capacity of the constitutive equations and the agreement between the predicted strain-time curves and experimental data has been evaluated.

2. Materials and methods

2.1. The θ-Projection

The θ-Projection method is based on Equation 1, in which the four parameters (θ_i, i = 1-4) are obtained from an experimental creep curve. The expression may be divided into two parts: i) the primary creep rate $\theta_1\left(1-e^{-\theta_2 t}\right)$, in which θ_1 represents the primary strain magnitude and θ_2, the decay rate; and ii) the accelerating creep rate $\theta_3\left(e^{\theta_4 t}-1\right)$, in which θ_3 refers to the scaling of the tertiary creep strain and θ_4, to its rate[12].

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Thus, θ_1 and θ_3 are denominated scale parameters, whereas θ_2 and θ_4, rate parameters[5].

$$\varepsilon = \theta_1\left(1 - e^{-\theta_2 t}\right) + \theta_3\left(e^{\theta_4 t} - 1\right) \quad (1)$$

2.2. ν Concept

The υ Concept considers the Continuous Damage Mechanics framework (CDM) (Equation 2). The υ parameters of this constitutive equation can be independently extracted from the creep curves, as reported in[3,6]. To predict the creep curve, the parameters ν_i (i = 1-4) and the fracture time (t_f) are considered. However, in this study, the values of υ and θ will be determined by a computational technique using six experimental curves[3,6].

$$\varepsilon = \nu_1\left(1 - e^{(-\nu_2 t)}\right) + \nu_3\left[1 - \left(1 - \frac{t}{t_f}\right)^{\nu_4}\right] \quad (2)$$

2.3. Time to rupture

Time to rupture must be calculated to predict creep curves. This parameter was used in both the θ-Projection and the ν Concept. The dependence of fracture time on applied stress is frequently described by an exponential fit curve (Equation 3) in which A and m are constants and σ, the applied stress.

$$t_f = A\sigma^m \quad (3)$$

2.4. Experimental data

To determine the four θ and ν values and further apply the θ-Projection and ν Concept methods, the experimental data of six creep curves were considered (Figure 1). These curves were previously obtained by Barboza[3] and Barboza et al.[6] using Ti-6Al-4V specimens with the following chemical composition: 6.61 Al – 4.23 V – 1.18 Fe – 0.13 O – 0.026 C – 0.011 N – 0.003 H – Ti. The microstructure is composed of an α-phase with an average grain size of 10 μm and a β-phase in the grain boundaries of α. The experiments were performed on a dead-weight-creep-rupture machine at six applied stress values (312 to 520 MPa) at 500 °C. Experimental data from a test performed at 465 MPa under the same conditions (not included in the estimation of θ and ν values) were used to compare the results obtained by the θ-Projection and ν Concept methods.

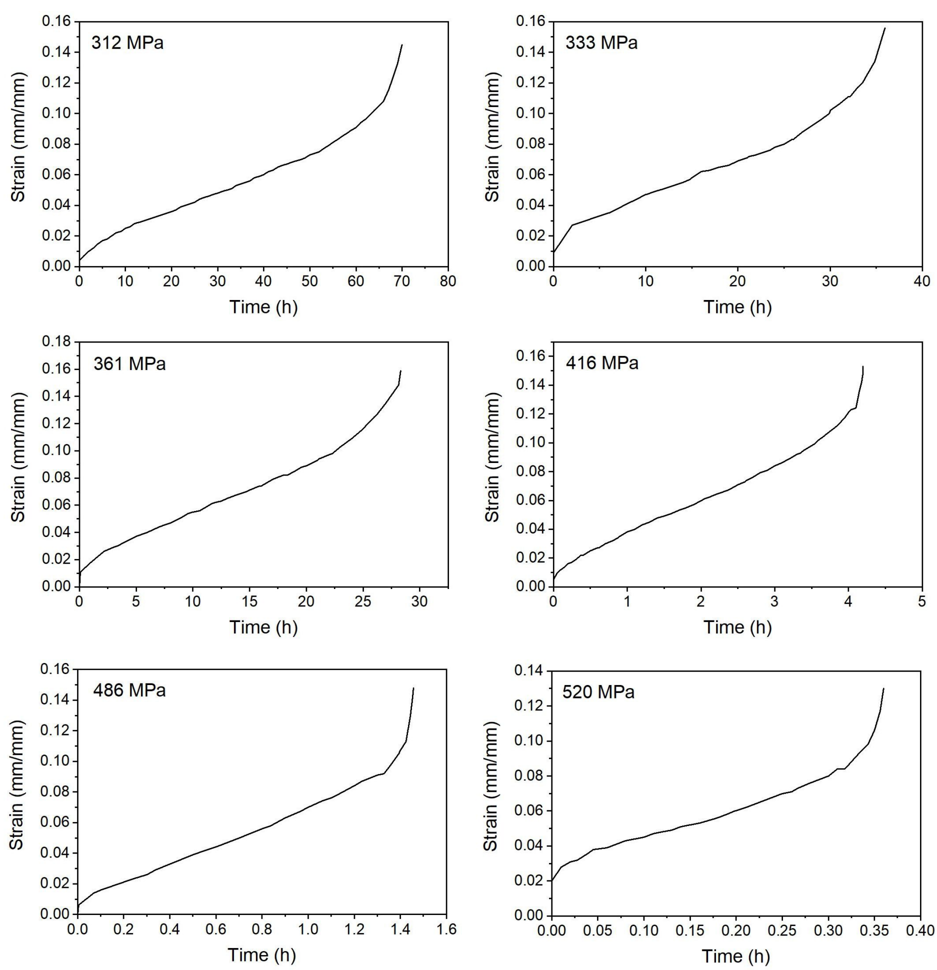

Figure 1. Ti-6Al-4V experimental creep curves (312 to 520 MPa) at 500 °C used to determine the θ and ν parameters[3,6].

Creep tests results (Figure 1) are summarized in Table 1, which shows rupture time (t_f), strain at fracture (ε_f) and the applied stress (σ)[3,6].

Table 1. Creep parameters at 500 ºC of Ti-6Al-4V[3,6].

σ [MPa]	t_f [h]	ε_f [mm/mm]
312	70.01	0.159
333	35.97	0.156
361	28.19	0.1581
416	4.20	0.153
486	1.47	0.148
520	0.36	0.130

2.5. The Software

A software was developed using the Python programming language to obtain creep curve data considering the θ-Projection and the ν Concept. This computational technique allowed obtaining the θ and ν parameters for a set of Ti-6Al-4V alloy curves, shown in Figure 1. The linear equations were obtained by plotting the experimental θ_{1-4} and υ_{1-4} values as a function of the applied stress and were further treated by the software Origin ® 2018 fit curve tool. The fracture time to predict the curve at 465 MPa was determined by entering the database (Equation 3) into the software. The equations 4-11 allowed interpolation to determine θ and ν values at 465 MPa. These values were implemented in Equations 1 and 2 and the time steps were varied by 0.1 h, enabling the prediction of the strain-time curve at 465 MPa. A flowchart summarizing the steps of this study is shown in Figure 2.

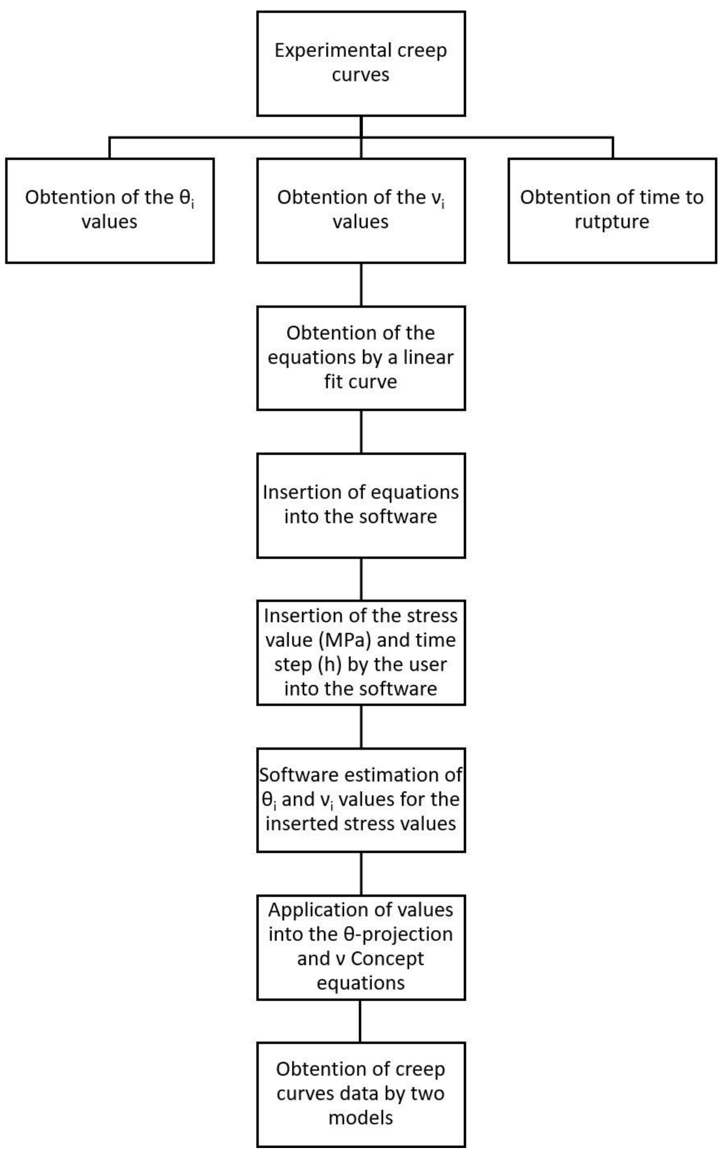

Figure 2. Flowchart describing the steps performed to predict creep curves following the θ-projection and ν Concept methodologies.

3. Results and Discussion

3.1. Short-term creep curve prediction by applying the θ-Projection and ν Concept

Based on creep curve data (Figure 1), θ and ν values were determined. Data are shown in Table 2 and plotted in Figure 3.

A linear regression was performed and represented by Equations 4-11, that enabled the extraction of parameters θ and ν at 465 MPa. These values are shown in Table 3.

$$ln(\theta_1) = -0.0006\ \sigma - 3.4763 \quad (4)$$

$$ln(\theta_2) = 0.0266\ \sigma - 10.076 \quad (5)$$

$$ln(\theta_3) = -0.0028\ \sigma - 1.1571 \quad (6)$$

$$ln(\theta_4) = 0.0248\ \sigma - 12.427 \quad (7)$$

$$ln(\nu_1) = 0.0005\ \sigma - 4.1723 \quad (8)$$

$$ln(\nu_2) = 0.0234\ \sigma - 8.2638 \quad (9)$$

$$ln(\nu_3) = -0.0009\ \sigma - 1.7263 \quad (10)$$

$$ln(\nu_4) = -0.0018\ \sigma + 0.0083 \quad (11)$$

Based on Table 1 data, time to rupture as a function of the applied stress (Figure 4) curve was plotted. Based on Equation 3 and standard regression techniques, A = 3.756 × 10^{26} and an m = −9.89 has been determined. At 465 MPa, rupture time corresponds to 1.6 h.

3.2. Use of the θ-Projection and ν Concept to predict creep curves at 465 MPa

The introduction the θ_i and ν_i values of Tables 2 and 3, the rupture time calculated by Equation 3 for 1.6h at 465 MPa,

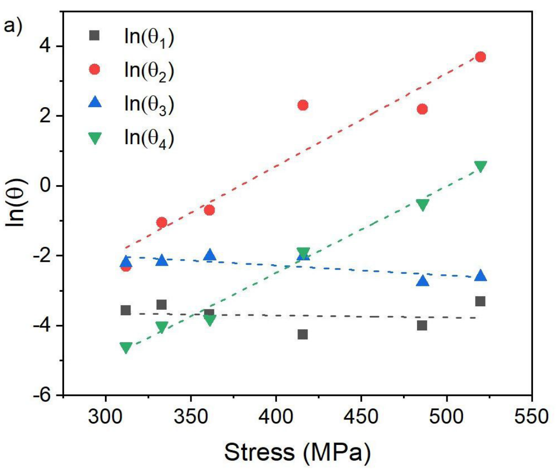

Figure 3. Dashed lines represent the linear regression performed in each point set: a) θ-Projection and (b) ν Concept.

Table 2. Values of $ln(\theta_i)$ and $ln(\nu_i)$ (i: 1- 4).

Stress (MPa)	θ-Projection				ν Concept			
	$\ln(\theta_1)$	$\ln(\theta_2)$	$\ln(\theta_3)$	$\ln(\theta_4)$	$\ln(\nu_1)$	$\ln(\nu_2)$	$\ln(\nu_3)$	$\ln(\nu_4)$
312	-3.58	-2.30	-2.21	-4.61	-4.27	-0.53	-2.04	-0.63
333	-3.41	-1.05	-2.17	-4.02	-3.65	-0.58	-2.05	-0.68
361	-3.69	-0.69	-2.01	-3.82	-3.91	-0.25	-2.00	-0.51
416	-4.27	2.30	-2.01	-1.90	-4.07	1.61	-2.12	-0.50
486	-4.02	2.20	-2.76	-0.51	-4.42	3.00	-2.04	-1.05
520	-3.32	3.69	-2.61	0.59	-3.51	4.09	-2.30	-0.88

Table 3. The θ and ν values obtained from Equations 4-11 at 465 MPa.

θ_1	θ_2	θ_3	θ_4	ν_1	ν_2	ν_3	ν_4
0.0234	9.9046	0.0855	0.4086	0.0195	13.6973	0.1171	0.4366

and the 0.1h time step in software, enabled creep curve prediction by the θ-Projection (Equation 1) and ν Concept (Equation 2) models. Figure 5 shows the software-derived data in comparison with an experimental curve at 465 MPa and a time to rupture of 1.92h. The percentage difference between times to rupture calculated by Equation 3 and the experimental value corresponds to 17%. The creep ductility of the experimental curve corresponds to 0.129. However, values obtained by the θ-Projection and ν Concept methods correspond to 0.103 and 0.137, respectively. Based on Figure 5, the tertiary stage is well defined by the ν Concept (Equation 2) with the typical curvature obtained for Ti-6Al-4V in tests under a constant load.

In general, creep curves have been described by few parameters, such as lifetime, rupture strain, and creep stationary rates. In this case, other information available from a creep curve is ignored. A complete description requires constitutive equations that can describe the normal creep curve under certain conditions of stress and temperature.

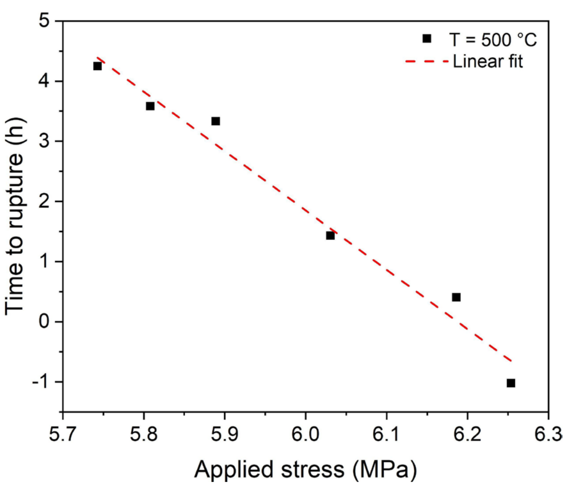

Figure 4. Dependence of time to rupture (h) on applied stress (MPa)[3,6].

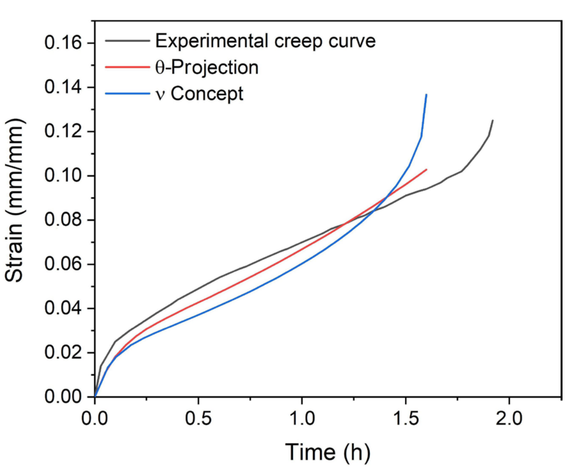

Figure 5. Creep curves calculated by Equations 1 and 2 and experimental data at 465 MPa.

The ν Concept and θ-Projection methodologies offer a description based on four ν_i and θ_i parameters, respectively. The ν_1, ν_2, θ_1, and θ_2 parameters represent the first and second creep stages; whereas the ν_3, ν_4, θ_3, and θ_4 parameters, the tertiary creep stage. These constitutive equations are based on strain hardening, recovery mechanisms, and creep damage[5,6]

This study obtained ν_i and θ_i parameters by computational techniques for uniaxial Ti-6Al-4V alloy creep test specimens. Such parameters depend on microstructure, applied stress and temperature. The technique is based on creating a database for a given material that allows the extrapolation or interpolation of creep curves[5,13,17]. In this case, the database presents six curves obtained at 500 ºC at 312 to 520 MPa for Ti-6Al-4V (Figure 1). Based on these six curves, θ_i and ν_i parameters were determined by the software developed in this work based on flowchart shown in Figure 2. The values are shown in Table 2 and Figure 3. These values enabled the prediction of the creep curve at 465 MPa. Regardless of the different strain and damage mechanisms, the linear configuration of ν_i and θ_i as a function of applied stress favors the interpolation process. Both methods have been shown to predict primary, secondary, and tertiary creep behavior for Ti-6Al-4V with acceptable accuracy (Figure 5). However, results indicated that the ν Concept produced a creep curve with better agreement with the experimental data.

As reported in[13], the θ-Projection has been widely used for modeling creep behavior under constant stress. Creep behavior under a constant load cannot be accurately describe, as observed in references[13,17] and in this work for Ti-Al-4V. In this context, other studies have been presented in the scientific literature to minimize the deviation of the predicted creep curves under constant load[13,17]. However, results indicated that the ν Concept produced a creep curve with better agreement with the experimental data. Such a fact is related to the combination of mathematical functions for the primary and tertiary regimes of the ν Concept, which result in better agreement for tests under constant load conditions.

4. Conclusions

This study developed a software for the direct application of the θ-Projection and ν Concept mathematical models to predict creep behavior. Results indicated that the ν Concept and θ-Projection models showed good agreement with the experimental data. Results indicated that the ν Concept produced a creep curve with greater agreement with the experimental data. Note that the ν Concept better defined the tertiary stage. Furthermore, more experimental data are needed to improve prediction agreement. Databases with ν and θ must be designed for other Ti-6Al-4V microstructures under different stress-temperature regimes. The technique used to obtain parameters is promising and should be improved for future studies.

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