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A Unified Mechanics Theory-Based Damage Model For Creep in Nickel-Based Superalloys

Sri Krishna Sudhamsu Kambhammettu[#,*], Saurabh Mangal[$], Lakshmana Rao C.[$] and Perumal Chellapandi[!]

[#]Department of Mechanical Engineering, NIT, Jamshedpur - 831 014, India
[$]Department of Applied Mechanics, IIT Madras, Chennai - 600 036, India
[!]BharatiyaNabhikiya Vidyut Nigam Limited (BHAVINI), Kalpakkam - 603 102, India
[*]E-mail: ksksudhamsu@gmail.com

ABSTRACT

Unified Mechanics Theory's (UMT) entropy-based damage parameter, also known as the "Thermodynamic State Index" has been proven to be consistent and useful in predicting the fatigue life of different metal alloys. In recent times, studies have also demonstrated its applicability towards creep damage in nickel-basedsuperalloys under a limited set of conditions. However, the usefulness of the "Thermodynamic State Index" in estimating damage at different temperatures, and creep loads for different metal alloys has not been evaluated yet. In this paper, creep in INCONEL 600 alloy is modeled using Norton's creep law modified with entropy-based damage (Thermodynamic State Index). The model is calibrated to predict both damage and creep strains for any given input of stress, temperature, and time. The available database on INCONEL 600 is used in parts to both calibrate and validate the prescribed model. The damage evolution for different cases is compared and imminent conclusions are drawn.

Keywords: Creep; High temperature; Unified mechanics theory; Entropy; Nickel-based superalloy

1. INTRODUCTION

Creep failure is one of the most commonly observed modes of failure in components that are employed at high homologous temperatures[1]. Such failure is generally estimated using continuum damage mechanics (CDM) models that rely on damage parameters to assess the proximity of the material to failure[2]. These damage parameters generally start from 0 (for the virgin material) and evolve to 1 at failure. The definition and the evolution of these parameters are generally obtained using empirical relations that satisfy the said criteria at 0 (start / virgin material) and 1(end/failure). Over decades, these parameters have proven to be very useful in assigning a meaningful number to an otherwise qualitatively understood term: damage. However, these damage parameters are defined differently for different failure modes such as creep, low-cycle fatigue, and high-cycle fatigue.

For example, the creep damage parameter[3] is defined by D and is given by Eqn. 1.

$$D = 1 - \left(1 - \frac{t}{t_r}\right)^{\frac{1}{\eta}+1} \tag{1}$$

where

t is the time for exposure for creep loading

t_r is the time for rupture at a given creep stress

η is a constant in the creep model

At the same time, the fatigue damage parameter in[4] is defined by D and is given by Eqn. 2.

$$D = \left(\frac{N}{N_f}\right)^f \tag{2}$$

where,

N is the number of load cycles applied on the material

N_f is the number of load cycles for rupture at a given creep stress

f is a material-dependentconstant

Firstly, since both these parameters are defined in different manners, same value of damage parameters, say for example, D=0.5 for creep and for fatigue does not imply the same state of damage for the material. Secondly, if creep and fatigue were to occur simultaneously, there is no direct way to integrate both parameters into one value that represents the overall damage state of the material. Finally, it is very difficult to define the evolution algorithm of such damage parameters in the event other loads/environmental conditions such as temperature and pressure are varied. For this reason, most damage parameters lack universality barring them from being employed for various loading conditions.

To address these shortcomings, unified mechanics theory[4] employs an entropy-based damage parameter (known as the Thermodynamic State Index (TSI)). This theory envisages damage as a culmination of all the irreversible, dissipative processes that occur in a material during its lifetime. Such irreversible processes would keep changing the microstructural arrangement of the material while simultaneously increasing the probability of complete disruption (functional failure/ material rupture) of such microstructural arrangement. This process ultimately leads to functional failure/ material rupture

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at any given material point of interest. The number of such irreversible processes/microstructural rearrangements that have occurred in the service time of the material can be measured using the entropy generated in the material during the same service time. A damage definition that is based on entropy only depends upon the second law of thermodynamics that determines the degradation in a system. For a given amount of entropy generated, such a definition is hence independent of the particular mechanisms that cause such entropy generation/ degradation. Equation 3 gives the damage parameter (also known as the Thermodynamic State Index (TSI)) defined by Unified Mechanics Theory.

$$\phi = \left(1 - e^{-\frac{m_s \Delta s}{R}}\right) \tag{3}$$

where

ϕ is the damage parameter or Thermodynamic State Index

Δs is the specific entropy generated at the material point of interest

m_s is the specific mass (gram/mole)

R is the universal gas constant

This damage definition has been successfully used to determine the damage state of a material undergoing a combination of degradation processes such as low cycle fatigue, high cycle fatigue, electro-migration, thermo-migration, and plastic deformation[5-7]. Some preliminary work has also been reported on modeling creep degradation using unified mechanics theory. In[8], the evolution of the Thermodynamic State Index (damage parameter) during creep degradation is investigated for solder alloys. Sudhamsu[9], *et al.* investigated the Thermodynamic State Index at the end of secondary creep for DZ-125 Nickel-based superalloy and reported that the TSI remains the same at the end of secondary creep irrespective of the creep stress applied on the material. In[10], Wang, *et al.* investigated the entropy at creep rupture for different metal alloys and reported that this value remains constantirrespective of the creep stress and creep temperature. In this paper, we attempt to build a basic damage mechanics model using a UMT-based damage parameter i.e. Thermodynamic State Index (TSI). We calibrate this model using a portion of the existing data on Inconel 600 and subsequently use this model to predict creep strain and damage state at various creep stresses, temperatures, and times. We also compare this data with the remaining portion of experimental data and evaluate the prediction accuracy. We later discuss the limitations of the developed model and the avenues for improvement of the model in general. The objectives of this paper are to

- Develop a damage mechanics-based creep estimation model using unified mechanics theory-based damage prediction
- Validate the predictions at different temperatures and creep stresses using experimental data available for Inconel 600
- Explore the limitations and set the path forward for improvement of the model.

2. MODEL FORMULATION

2.1 Evaluation of Thermodynamic State Index (i.e. The Damage Parameter

To evaluate the Thermodynamic State Index, the definition presented in Eqn. 3 is followed. The main challenge, however, in using this definition stems from estimating the amount of entropy generated due to various degradation processes. Such relations that determine the entropy generation due to low cycle fatigue, high cycle fatigue, electro-migration, thermo-migration, and plastic deformation are already established[5-7]. However, such studies have not yet been done for creep deformation. Creep deformation is often found to occur due to (a) dislocation movement (primary creep) (b) diffusion (secondary creep) and (c) grain boundary sliding (tertiary creep). These phenomena occur at different stages of creep deformation of a material/specimen as shown in Fig. 1.

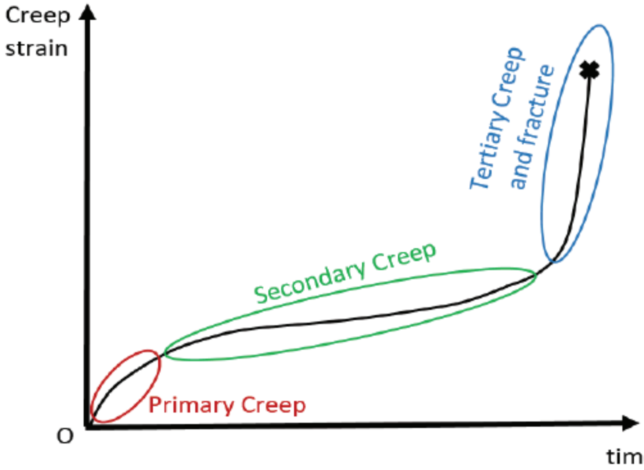

Figure 1. A schematic showing creep zones in a typical creep curve.

To correctly find out the entropy generated in creep, entropy generated due to all these three phenomena should be estimated accurately. In the absence of such equations that describe each of the relevant mechanisms, it is possible to estimate entropy generated in the material by carefully monitoring the work and energy transactions between the material and the surroundings. A major chunk of energy dissipated (by the material) during creep deformation comes from the work done by the creep load on the material. In this paper, as a first approximation, we consider entropy generated due to the inelastic work done on the material as the cause of entropy generation during creep deformation. Consequently, the entropy relation shown by Eqn. 4 is obtained.

$$\Delta s = \int_{t_1=0}^{t_2} \sigma \, \dot{\varepsilon}^c \, dt \tag{4}$$

Entropy generated (due to inelastic work done on the material/ due to energy dissipation in the material) beyond a certain threshold is assumed to alter the overall arrangement of the atoms to such an extent that makes it unfit for any further usage (failure). This limits the maximum value of the Thermodynamic State Index (ϕ) attainable by a material.

2.2 Constitutive Relations

For modeling creep, we require two constitutive relations: One, is the stress-strain relation that provides the instantaneous response in elastic region. Two, the creep strain-stress-time relation that provides the long-term creep response. In this section, we write these equations for one-dimensional loading and degrade the known parameters as the damage takes place. However, the process can be adopted for a general state of stress by bringing in the concept of equivalent strain whenever and wherever needed.

Consider a rod of uniform cross-section pulled by a constant force P (resulting in auniaxial-stress of magnitude σ). The true stress in the material is a result of its elastic deformation and is given by Hooke's law. This stress (σ) is given by

$$\sigma = E'\varepsilon^{e} \tag{5}$$

where

E' is effective elastic modulus which is related to the damage parameter, TSI by $E' = E(1-\phi)$

E is elastic modulus of the material

ε^{e} is the elastic strain which is given by $\varepsilon^{e} = \varepsilon - \varepsilon^{C}$

ε^{C} is creep strain and ε is total strain

Hence,

$$\sigma = E(1-\phi)(\varepsilon - \varepsilon^{c}) \tag{6}$$

Depending on the material and the loading conditions in hand, other relations may be used. For describing creep, in this paper, we utilize Norton's law for creep. Norton's law is known for its simplicity and its accuracy in describing secondary creep and tertiary creep. Nickel-based superalloys are known for their extended tertiary creep zone and small primary creep zone. Hence, it is convenient for us to start with this creep law. This creep law is given by the equation

$$\dot{\varepsilon}^{c} = A\sigma^{n} e^{-\frac{Q}{RT}} \tag{7}$$

where

$\dot{\varepsilon}^{c}$ is creep strain rate

Q is diffusion creep activation energy

A and n are model parameters

The equations describing the Thermodynamic State Index and entropy evolution are given by Eqn. 3 and Eqn. 4 respectively and are reproduced by Eqn. 8 and Eqn. 9 for the sake of convenience of the reader.

$$\phi = \left(1 - e^{-\frac{m_s \Delta s}{R}}\right) \tag{8}$$

$$\Delta s = \frac{1}{\rho T}\int_{t_1=0}^{t_2} \sigma\, \dot{\varepsilon}^{c} dt \tag{9}$$

For a given creep loading $\sigma(t)$, in the above equations, we have four unknowns: total strain ($\varepsilon(t)$), creep strain ($\varepsilon^{C}(t)$), entropy generated ($\Delta s(t)$) and Thermodynamic State Index ($\phi(t)$). We also have four independent equations (Eqn. 6,7,8 and 9) that should allow for solving them simultaneously to find all the four unknowns.

We eliminate ε^{C}, Δs and ϕ to get Eqn. 10

$$\varepsilon = \frac{\sigma}{E\left(e^{-\frac{m_s \frac{1}{\rho T}\int_0^t \left(A\sigma^{n+1} e^{-\frac{Q}{RT}}\right)dt}{R}}\right)} + \int_0^t A\sigma^{n} e^{-\frac{Q}{RT}} dt \tag{10}$$

The above equation shows that the total strain is the sum of the elastic strain component of the damaged material (1st term) and creep strain (2nd term).

2.3 Parameter Estimation for Inconel 600

To fit the unknown parameters for any given material, we need time-stress-strain data from a uniaxial tensile/compressive creep test at different applied creep stresses (engineering stresses) and temperatures. In this paper, we utilize the creep data for Inconel 600 alloy from Chavez[11], *et al.* We consider the data at three different creep engineering stress and temperature pairs: (71 MPa, 1144 K), (55 MPa, 1144 K), and (137 MPa, 1005 K). We evaluate the true stress and true strain at every data point using engineering stress and engineering strain. This will allow us to get a discrete data (σ,ε,t) at different times t ranging from t=0 to $t=t_r$ (time for rupture), we define a function $f(A,n,Q)$ using equation-10 which has to be zero at every data point (σ,ε,t).

$$f(A,n,Q) = \varepsilon - \frac{\sigma}{E\left(e^{-\frac{m_s \frac{1}{\rho T}\int_0^t A\sigma^{n+1} e^{-\frac{Q}{RT}}dt}{R}}\right)} - \int_0^t A\sigma^{n} e^{-\frac{Q}{RT}} dt \tag{11}$$

We minimize the squared sum of this function at every data point ($f^2(A,n,Q)$) to find out the optimized values of A, n and Q. We perform this using lsqnonlin command in MATLAB (which uses Levenberg-Marquardt algorithm for the optimization). The values of A, n and Q for the given data are found to be $A=4.4\times10^{-17}$, n=3.36 and Q=240000 in S.I. units. The calibrated model is now used to predict the creep strain - time curves (using Eqn. 10) at different creep stresses and temperatures. The creep activation energy thus fit is found to be well within the range observed in the literature[12].

3. RESULTS AND DISCUSSION

Figures 2,3,4 and 5 show the strain-time and strain rate–time curves at different applied creep stresses and temperatures. To evaluate the effectiveness of prediction, we define the absolute percentage error in estimating the creep strain at any given time 't' from the start of the creep experiment. This is shown by Eqn. 12.

$$e_p(\sigma,t) = \left|\frac{\varepsilon_p(\sigma,t) - \varepsilon_e(\sigma,t)}{\varepsilon_e(\sigma,t)}\right| x100 \tag{12}$$

where

e_p is the percentage error

ε_p is predicted strain

ε_e is a strain observed experimentally

The mean and standard deviation of such error percentages evaluated for the range of creep stress and creep strain data at each temperature is shown in Table 1 It can be observed that there is a decent match between the predictions and the experiments despite using the same model parameters across temperatures and creep loads. For all the temperatures and stresses, an initial decrease followed by a rapid increase in creep strain rate can be observed from the experimental data. This initial decrease characterizes the primary creep region. The estimated curves do not show any such feature. This is because Norton's creep law is only capable of describing secondary and tertiary creep. However, this is acceptable to us as the extent of creep in the primary creep region is small. In cases where substantial primary creep is observed, a different creep law but with the same damage parameter i.e. Thermodynamic State Index (TSI) could be used. The development of model equations in such a case would be very similar to that shown in this paper.

Table 1. Magnitude of errors associated with prediction

Temperature (T)	Mean percentage error (%)	The standard deviation of mean percentage error
1005	5.8	6.5
1144	2.7	3.0
1255	15.7	16.8
1376	7.8	7.8

For all engineering purposes, creep failure is defined to occur once a material reaches the tertiary creep zone. This transition is nearly around the same location as that of the end of the minimum strain rate zone. The damage parameter (or the Thermodynamic State Index) calculated at the end of the secondary zone for various stress and temperature values is shown in Table2. The value of this parameter can be estimated

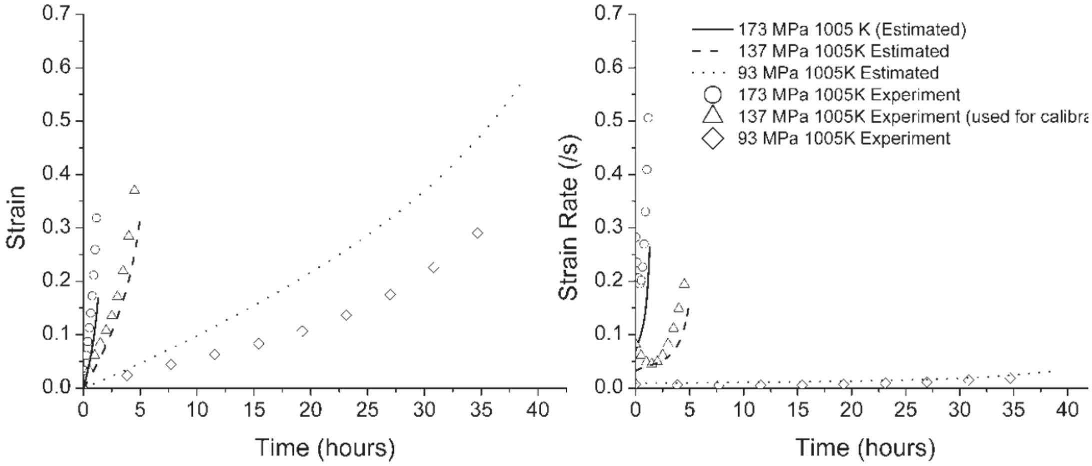

Figure 2. Strain- time and strain rate - time curves at different creep (engineering) stresses at 1005K.

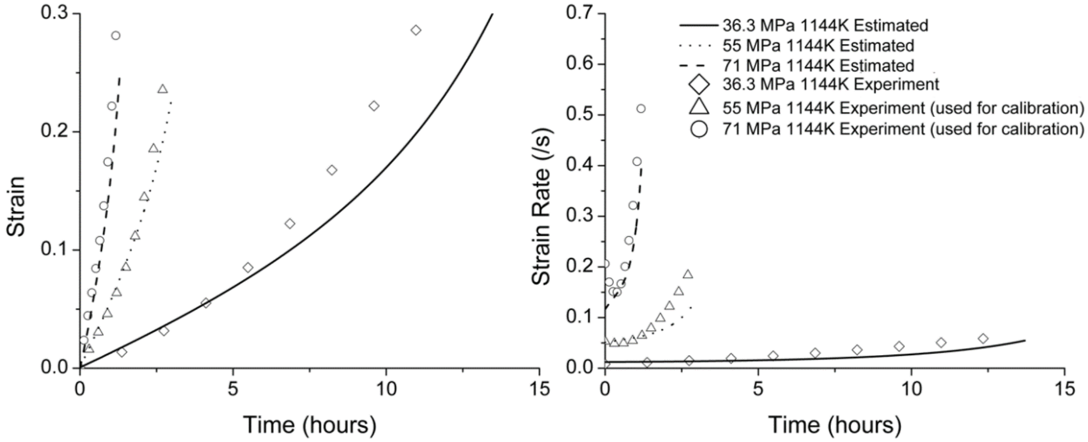

Figure 3. Strain- time and strain rate - time curves at different creep (engineering) stresses at 1114 K.

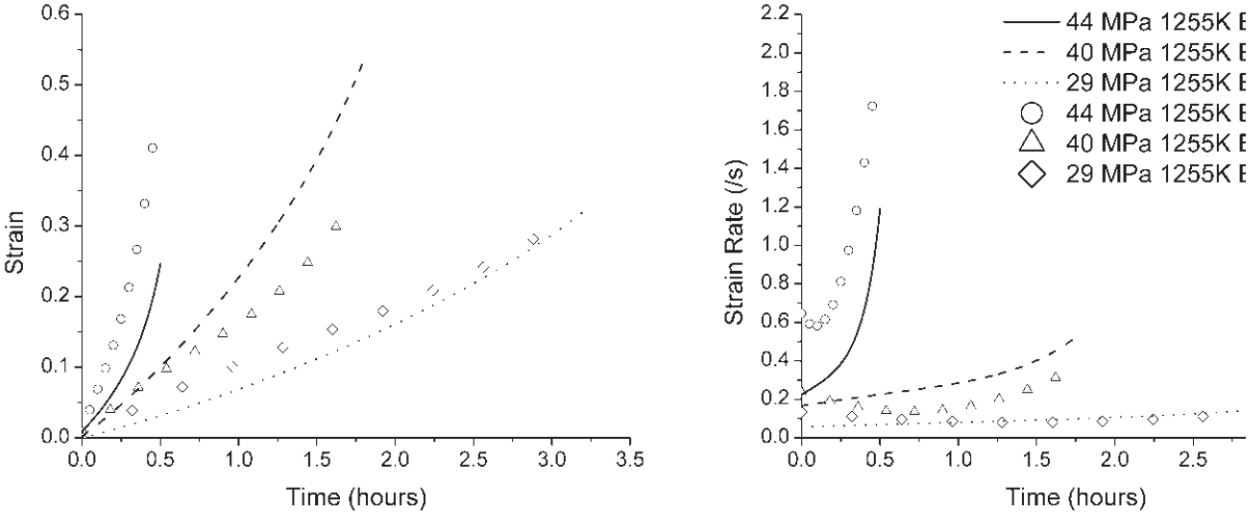

Figure 4. Strain- time and strain rate - time curves at different creep (engineering) stresses at 1255K.

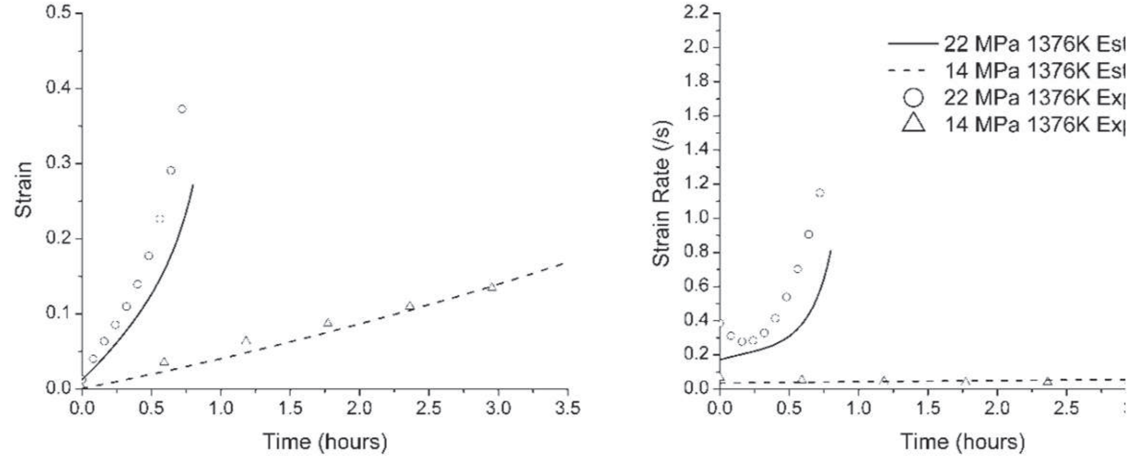

Figure 5. Strain- time and strain rate - time curves at different creep (engineering) stresses at 1376 K.

Table 2. Thermodynamic State Index at different creep stresses and temperatures

Temperature (K)	Creep stress (MPa)	TSI at the beginning of tertiary creep
1005	173.2	0.013
1005	137.8	0.013
1005	93.6	0.013
1144	71.2	0.011
1144	71.1	0.011
1144	55.6	0.007
1144	36.1	0.007
1255	44.1	0.008
1255	40.6	0.016
1255	29.5	0.018
1376	22.2	0.011
1376	14.1	0.013

using Eqn. 3 and Eqn. 4. We expect that the TSI at the end of secondary creep will be the same irrespective of the creep stress and temperature under consideration. It can be observed from Table 2 that the TSI is more or less constant at each temperature but varies from temperature to temperature. This indicates that there are other sources of entropy generation other than the dissipation through creep work. The authors believe that the major possible source of such entropy generation is the entropy generated due to heat dissipation in the material. Since no such thermal data is available from creep experiments, the entropy generated due to such dissipation cannot be estimated in this way. However, one can model the basic mechanisms of creep such as diffusion and grain boundary sliding to estimate the entropy generated more accurately. Such treatment is beyond the scope of the present work and will be taken up subsequently.

4. SUMMARY AND CONCLUSIONS

In this paper, a unified mechanics theory-based CDM approach to estimate creep across temperatures and creep loads in metal alloys is presented. The CDM model is used to describe already conducted experiments on INCONEL-600. The model uses an entropy-based damage parameter known as the Thermodynamic State Index (TSI) to track the "damage state" of the given material. In this treatment, Norton's creep law is used to characterize the creep constitutive relation. However, the same treatment of entropy-based damage can be extended to other creep laws as well as per the requirement. The creep strain thus estimated using this model largely agreed with the creep strains observed in the experiment. However, noticeable differences in the Thermodynamic State Index were observed at different temperatures. This is attributed to the other sources of entropy that are not considered in this paper. A more detailed development with modeling of mechanisms is required to conclusively verify the uniqueness of the Thermodynamic State Index (TSI) as the sole damage parameter. This will be taken up by the authors subsequently.

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CONTRIBUTORS

Dr Sri Krishna Sudhamsu Kambhammettu is an Assistant Professor at National Institute of Technology Jamshedpur. He works in the general area of solid mechanics with a focus on engineering applications pertaining to specific areas such as damage mechanics, impact mechanics and sealing technology. For this work, he contributed to conceptualization, methodology, formal analysis,, software, writing-original draft preparation and writing-review & editing and supervision.

Mr Saurabh Mangal is an MS Research Scholar at the Department of Applied Mechanics, Indian Institute of Technology Madras. He completed his BTech in Mechanical Engineering from Rajasthan Technical University. His area of research includes material modelling, finite element analysis, numerical simulations, creep, fatigue, creep-fatigue interaction, etc.
For this work, he contributed to conceptualization, analytical formulations, investigation, methodology, validation, data curation, formal analysis and writing-review & editing.

Dr Lakshmana Rao C. is a Professor in the Department of Applied Mechanics at IIT Madras. He has obtained his bachelor's and master's degrees from the Department of Civil Engineering at IIT Madras and DS in mechanics of materials from Massachusetts Institute of Technology. His areas of specialisation include solid mechanics in general and damage mechanics, impact mechanics, fracture mechanics and finite element analysis in particular.
For this work, he contributed to analytical investigation, resources, writing-review & editing and supervision.

Dr Perumal Chellapandi is a Distinguished alumnus of IIT Madras with MTech and PhD in Applied Mechanics. He got his DS from AMET University, Chennai. He is a Fellow of Indian National Academy of Engineering. Currently, he is an INAE Distinguished Professor at IIT-Madras Chennai. His major specialisations are Fast Reactor Design & technology in general and High-temperature design and fast transient fluid-structure interaction dynamic in particular.
For this work, he contributed to analytical investigation, resources, writing-review & editing and supervision.