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## **Bachelor Thesis**

in Mechanical Engineering, Vietnamese-German University

# **A parametric study for a toy model prescribing microstructure evolution under phase-transformation combined with plasticity**



Vietnamese-German University

**Truong Duc Minh**

Matr.-Nr. 1080 20263309

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**Supervisor(s):**

Prof. Dr. Klaus Hackl  
Institute of Mechanics of Materials  
Ruhr University Bochum

Ghina Jezdan  
Institute of Mechanics of Materials  
Ruhr University Bochum

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A handwritten signature in black ink, appearing to read 'Dml', is written over a horizontal line. The signature is fluid and cursive.

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Tuesday, November 14, 2023

**Frequently used Greek symbols**

$\psi$	Helmholtz free energy
$\varepsilon$	Strain
$\sigma$	Stress
$\alpha$	Hardening parameter
$\beta$	Hardening parameter
$\eta$	Viscous parameter
$\gamma$	Viscous parameter
$\Delta$	Dissipation potential
$\lambda$	Volume fraction

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## 1. Introduction

Material behaviour under deformation has always been a great concern to both scientific and engineering worlds. One of the most well-known and deeply researched behaviour under deformation is plasticity, which is the irreversible deformation of the material under macroscopic scale. Research have been conducted both experimentally and theoretically in order to deeply understand this phenomenon, as this awareness would provide engineers with the capability of understanding material behaviour under deformation as well as under different loading conditions. Usually, theoretical approach would aim at studying material states under microscopic level, as per the fact that, material reaction in macroscopic scale is the reflection of what is occurring in the microscale. These states can be described via continuum mechanics and thermodynamics, with the aid of material internal variables and material parameters. This paper aims at providing a miniature study on a one-dimensional elasto-viscoplastic material with isotropic hardening under microstructure evolution, particularly focusing on how material parameters would influence on the material behaviour. In this paper, we first have an overview of the general theory that prescribes the phenomenon as well as coming up with the evolution equations of the internal variables. We then propose a computational approach which is based on the Forward-Euler scheme that can be applied on the equations that come along with the theory. Finally, we investigate separately the material parameters in a certain range, which will be mentioned later, and have a small discussion on the influence of each parameter alongside the result.

## 2. Theoretical basis

Plasticity, also known as plastic deformation, is a well-known mechanical phenomenon and has been extensively studied in research conducted worldwide. When a solid material undergoes tension (or compression), it exhibits deformation. This deformation remains reversible as long as the applied stress remains below a specific threshold, known as yield strength. The deformation is considered reversible, or in other words, elastic, when the material returns to its original shape once the loading is removed (Sadd, n.d.). However, once the material is stressed beyond the aforementioned elastic limit, the specimen will no longer recover its very original shape and dimensions. The strain retained by the specimen after it has

been fully unloaded is known as plastic deformation (Lubliner, 1990). In microscopic scale, this plastic deformation can be observed under the form of lattice defects, known as dislocations, through the crystal, which leads to the change of material's microstructure (Kochmann & Hackl, 2011a). In order to describe and evaluate the state of the microstructure, one can utilize the so-called internal variables, as well as material parameters. As a result, being able to evaluate material's internal variables also means the capability of predicting evolution of material's microstructure, which reflects plastic behaviour in macroscopic scale. One of the common approaches to study the evolution of internal variables is via variational principles resting on thermodynamic laws, such as the principle of maximum dissipation or the principle of minimum dissipation potential. Hackl and Fischer (2008) have noted that, compared to the principle of maximum dissipation, the principle of minimum dissipation potential is a pure minimization principle, thus it is more appealing with regard to describing the onset of microstructure evolution. The principle of minimum dissipation potential originates from Hamilton's principle, which is very handy in finding the actual motion of a system. Generally, the principle of minimum dissipation reads:

$$\dot{z} = \arg \min \{L(\phi, z, \dot{z})\}, \quad (1)$$

with the introduction of the Lagrange functional:

$$L = \dot{\psi}(\nabla \phi, z) + \Delta(z, \dot{z}), \quad (2)$$

where  $\psi$  stands for the Helmholtz free energy, which is dependent on deformation gradient  $\nabla \phi$  and the set of internal variables  $z$ , as well as  $\Delta$  being the dissipation potential. The dot ( $\dot{\cdot}$ ) denotes full derivative with respect to time. As stated in (1), minimizing Lagrange functional  $L$  would yield the evolution equations of the internal variables. In homogenous deformation, the Helmholtz free energy  $\psi$  is convex, thus minimization of  $L$  could be performed straight away, hence internal variables evolution equations would be well defined. However, the situation is not always this appealing, but rather in the other way around. Experimental findings show that usually a material would accommodate a macroscopic deformation by microstructural patterns, which could be a mix of homogeneous states with different minimal energy. It has even been concluded by Ericksen (1975), that microstructural patterns are the direct result of energy minimization. The appearance of the mixture of many energy dwells would create a fluctuation regarding the calculation of internal variables. In order to cope with the problem, convexification can be applied to the Helmholtz free energy. This study

approaches the case of one dimensional elasto-viscoplastic material with isotropic hardening, where a situation involving 2 phases of inelasticity, besides the pure elastic region, is considered.

General definition of the Helmholtz energy for a material was already mentioned by Coleman & Gurtin, (1966). Within the scope of this study, which is a one-dimensional situation, the Helmholtz free energy for elastoplastic material with isotropic hardening is given for each phase as:

$$\psi_1(\varepsilon_1, \varepsilon_{p1}) = \frac{c}{2}(\varepsilon_1 - \varepsilon_{p1})^2 + \frac{\alpha_1}{2}(\varepsilon_{p1})^2, \quad (3)$$

$$\psi_2(\varepsilon_2, \varepsilon_{p2}) = \frac{c}{2}(\varepsilon_2 - \varepsilon_{p2} - \varepsilon_T)^2 + \frac{\alpha_2}{2}(\varepsilon_{p2})^2 + c_T, \quad (4)$$

where  $\varepsilon_1, \varepsilon_2$  stand for overall strains in phases 1 and 2 respectively, and these are controllable external variables. Plastic strains  $\varepsilon_{p1}, \varepsilon_{p2}$  play the role of internal variables, which are uncontrollable and describe the state of the microstructure.  $c$ ,  $\alpha_1$  and  $\alpha_2$  denote the elastic moduli and hardening parameters of the 2 phases accordingly. There also exists a transformation parameter  $c_T$  and a transformation strain  $\varepsilon_T$  which are responsible for the transition to phase 2. According to Dacorogna (2008), convexification techniques can be applied to attain a relaxed energy, giving the relaxed energy as follow:

$$\psi_{mix}(\varepsilon, \varepsilon_{p1}, \varepsilon_{p2}, \lambda) = \inf \left\{ (1-\lambda)\psi_1(\varepsilon_1, \varepsilon_{p1}) + \lambda\psi_2(\varepsilon_2, \varepsilon_{p2}, \varepsilon_T) \mid \varepsilon_1, \varepsilon_2; \varepsilon = (1-\lambda)\varepsilon_1 + \lambda\varepsilon_2 \right\} \quad (5)$$

, where we distinguish between each evolving phase and its corresponding internal variables, therefore we introduce another internal variable, which is the volume fraction of the second phase  $\lambda$ , hence the corresponding volume fraction of the first phase is  $1-\lambda$ . Here, according to Hackl and Kochmann (2011),  $\lambda$  and  $1-\lambda$  are the probability distributions of the 2 phases observed from the microstructure. This statistical measure  $\lambda$  defines on which state the plastic evolution is acting. We can now also define the overall deformation  $\varepsilon$  as an average of the strains in both phases:

$$\varepsilon = (1-\lambda)\varepsilon_1 + \lambda\varepsilon_2, \quad (6)$$

The relaxed Helmholtz energy  $\psi_{mix}$  can finally be derived in a calculatable way, as:

$$\Psi_{mix}(\varepsilon, \varepsilon_{p1}, \varepsilon_{p2}, \lambda) = \frac{c}{2} \left[ \varepsilon - (1-\lambda)\varepsilon_{p1} - \lambda\varepsilon_{p2} - \lambda\varepsilon_T \right]^2 + (1-\lambda) \frac{\alpha_1}{2} (\varepsilon_{p1})^2 + \lambda \frac{\alpha_2}{2} (\varepsilon_{p2})^2 + \lambda c_T, \quad (7)$$

The next step is to define the relaxed dissipation potential. The total dissipation potential is considered to be made up of three parts: 1) the dissipation accounts for local evolution of visco-plastic strains with rate-independent and rate-dependent terms, 2) the phase change dissipation element, and 3) the dissipation due to jump in plastic strains. The three dissipation segments can be found as:

$$\Delta_1 = (1-\lambda) \left[ r |\dot{\varepsilon}_{p1}| + \frac{1}{2\eta} |\dot{\varepsilon}_{p1}|^2 \right] + \lambda \left[ r |\dot{\varepsilon}_{p2}| + \frac{1}{2\eta} |\dot{\varepsilon}_{p2}|^2 \right], \quad (8)$$

$$\Delta_2 = \frac{1}{2\gamma} \dot{\lambda}^2, \quad (9)$$

$$\Delta_3 = |\varepsilon_{p2} - \varepsilon_{p1}| \left( r |\dot{\lambda}| + \frac{\beta}{2\eta} \dot{\lambda}^2 \right), \quad (10)$$

the sum of which make the total relaxed dissipation potential:

$$\begin{aligned} \Delta_{mix}(\varepsilon_{p1}, \dot{\varepsilon}_{p1}, \varepsilon_{p2}, \dot{\varepsilon}_{p2}, \lambda, \dot{\lambda}) = & (1-\lambda) \left[ r |\dot{\varepsilon}_{p1}| + \frac{1}{2\eta} |\dot{\varepsilon}_{p1}|^2 \right] + \lambda \left[ r |\dot{\varepsilon}_{p2}| + \frac{1}{2\eta} |\dot{\varepsilon}_{p2}|^2 \right] + \frac{1}{2\gamma} \dot{\lambda}^2 \\ & + |\varepsilon_{p2} - \varepsilon_{p1}| \left( r |\dot{\lambda}| + \frac{\beta}{2\eta} \dot{\lambda}^2 \right) \end{aligned} \quad (11)$$

Within the dissipation potential we take into account two viscous parameters,  $\eta$  and  $\gamma$ , as well as threshold for plasticity  $r$  and a hardening parameter  $\beta$ , all of which stands for the material characteristics and are studied in the parametric study section of the paper.

It is well-known that minimizing the Lagrange functional would yield the actual motion of a mechanical system, in accordance with Hamilton's principle (Bedford, 2021). The same idea is applied to nonconservative systems characterized with internal variables. In order to obtain the evolution equations of the internal variables, one would minimize the Lagrange functional with respect to the rate of change of these internal variables respectively, which can be depicted mathematically as:

$$\frac{\partial \Psi_{mix}}{\partial \varepsilon} \dot{\varepsilon} + \frac{\partial \Psi_{mix}}{\partial \varepsilon_{p1}} \dot{\varepsilon}_{p1} + \frac{\partial \Psi_{mix}}{\partial \varepsilon_{p2}} \dot{\varepsilon}_{p2} + \frac{\partial \Psi_{mix}}{\partial \lambda} \dot{\lambda} + \Delta_{mix} \xrightarrow{\min_{\dot{\lambda}, \dot{\varepsilon}_{p1}, \dot{\varepsilon}_{p2}}}, \quad (12)$$

According to the 2<sup>nd</sup> law in thermodynamics, the partial derivatives of the Helmholtz free energy with respect to the internal variables signify the thermodynamic driving forces, which are stress-like constituents:

$$\frac{\partial \psi_{mix}}{\partial \varepsilon} = \sigma, \quad (13)$$

$$\frac{\partial \psi_{mix}}{\partial \varepsilon_{p1}} = -q_1, \quad (14)$$

$$\frac{\partial \psi_{mix}}{\partial \varepsilon_{p2}} = -q_2, \quad (15)$$

$$\frac{\partial \psi_{mix}}{\partial \varepsilon_\lambda} = -q_\lambda, \quad (16)$$

Performing the minimizations as given in (12) yields three differential equations, the so-called evolution equations for the internal variables, given respectively as follows:

$$0 \in \frac{\partial \psi_{mix}}{\partial \varepsilon_{p1}} + \frac{\partial \Delta_{mix}}{\partial \dot{\varepsilon}_{p1}}, \quad (17)$$

$$0 \in \frac{\partial \psi_{mix}}{\partial \varepsilon_{p2}} + \frac{\partial \Delta_{mix}}{\partial \dot{\varepsilon}_{p2}}, \quad (18)$$

$$0 = \frac{\partial \psi_{mix}}{\partial \lambda} + \frac{\partial \Delta_{mix}}{\partial \dot{\lambda}}, \quad (19)$$

The subdifferential symbol ( $\in$ ) is utilized as the continuity of the free energy term and the mix dissipation potential is not guaranteed, however the continuity character is not strictly required. Ultimately, solving the evolution equations (17), (18) and (19) respectively for the internal variables give:

$$\dot{\varepsilon}_{p1} = \eta \left[ c\varepsilon_{eff} - \alpha_1 \varepsilon_{p1} \mid -r \right] \text{sign}(c\varepsilon_{eff} - \alpha_1 \varepsilon_{p1}), \quad (20)$$

$$\dot{\varepsilon}_{p2} = \eta \left[ c\varepsilon_{eff} - \alpha_2 \varepsilon_{p2} \mid -r \right] \text{sign}(c\varepsilon_{eff} - \alpha_2 \varepsilon_{p2}), \quad (21)$$

$$\dot{\lambda} = \frac{\eta\gamma}{\eta + \gamma\beta|\varepsilon_{p2} - \varepsilon_{p1}|} \left[ \left[ c\varepsilon_{eff}(\varepsilon_{p1} - \varepsilon_{p2} - \varepsilon_T) - \frac{\alpha_1}{2}(\varepsilon_{p1})^2 + \frac{\alpha_2}{2}(\varepsilon_{p2})^2 + c_T \right] - r|\varepsilon_{p2} - \varepsilon_{p1}| \right] \text{sign}(q_\lambda), \quad (22)$$

It is also note-worthy that the yield functions, which are  $|c\varepsilon_{eff} - \alpha_i\varepsilon_{pi}| - r$  for  $\varepsilon_{pi}$  for  $i = 1, 2$ , and  $\left| c\varepsilon_{eff}(\varepsilon_{p1} - \varepsilon_{p2} - \varepsilon_T) - \frac{\alpha_1}{2}(\varepsilon_{p1})^2 + \frac{\alpha_2}{2}(\varepsilon_{p2})^2 + c_T \right| - r|\varepsilon_{p2} - \varepsilon_{p1}|$  for  $\lambda$  must be positive, as per the Kuhn-Tucker conditions, otherwise the internal variables would not evolve.

### 3. Computational approach

The aforementioned evolution equations of the internal variables are, however, analytically unsolvable due to the fact that these internal variables are well coupled, as well as them being differential equations that are dependent on the previous step values. In order to compute these equations in numerical scheme, we apply a time dependent incremental strain load, as well as introducing time increment  $\Delta t = t_{n+1} - t_n$ , thus solving the coupled problem. The mathematical formulation of the time increment implies that it has a step-wise even manner. Accordingly, an incremental increase of strain is applied to the system in order to examine the material behaviour. The time dependent overall strain reads:

$$\varepsilon^{n+1} = \bar{\varepsilon} \cdot t, \quad (23)$$

in which  $\bar{\varepsilon}$  stands for the rate of change of the overall strain  $\varepsilon$ .

However, there is still an unsolved problem, which is that the internal variables are still coupled. From equation (22), it is obvious that, without the initiation of either  $\varepsilon_{p1}$  or  $\varepsilon_{p2}$ , the volume fraction  $\lambda$  will never evolve. In order to untie the knot, one can maximize the driving force of  $\lambda$  with respect to  $\varepsilon_{p2}$  whilst keeping volume fraction of the second phase  $\lambda$  at zero, as Hackl and Kochmann have mentioned in their research (Kochmann & Hackl, 2011b). Within the scope of this study, the mentioned idea brings about the initial value of  $\varepsilon_{p2}$ :

$$\left. \frac{\partial q_\lambda}{\partial \varepsilon_{p2}} \right|_{\lambda=0} = 0, \quad (24)$$

which eventually yields the essential value  $\varepsilon_{p2,ini}$  :

$$\varepsilon_{p2,ini} = \frac{c}{\alpha_2} (\varepsilon - \varepsilon_{p1}), \quad (25)$$

In time incremental manner, this, indeed, is equivalent to:

$$\varepsilon_{p2,ini}^{n+1} = \frac{c}{\alpha_2} (\varepsilon^{n+1} - \varepsilon_{p1}^n), \quad (26)$$

It is also very note-worthy that, at the very beginning step of plasticity  $n + 1$ ,  $\varepsilon_{p1}^n$  is equal to zero, as so the other internal variables.



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Another issue which came about alongside with the initiation point, is a reference point of overall strain where plasticity occurs. This reference point can be understood as follow: as long as the overall strain is less than this value, the material is still well within elastic phase. One can find this reference point by setting the driving force of volume fraction  $q_\lambda$  to zero and substituting  $\varepsilon_{p2}^n$  with the value of  $\varepsilon_{p2,ini}^n$ , which, in a time increment setting, would eventually give:

$$\varepsilon_{ini}^{n+1} = \varepsilon_{p1}^n + \frac{\alpha_2}{c} \left[ (\varepsilon_{p1}^n - \varepsilon_T) + \sqrt{(\varepsilon_{p1}^n - \varepsilon_T)^2 - \frac{2}{\alpha_2} \left( \frac{\alpha_1}{2} (\varepsilon_{p1}^n)^2 - c_T \right)} \right], \quad (27)$$

With all obstacles resolved, we can now start the algorithm for material calculation. As per time increment setting, all the aforementioned equations will be modified with respect to this manner. The algorithm runs as follow:

**Algorithm:**

Time increment:  $\Delta t = t_{n+1} - t_n$

$$t = n\Delta t$$

Overall strain increment:  $\varepsilon^{n+1} = \bar{\varepsilon} \cdot t$

Compute  $\varepsilon_{ini}^{n+1, tr}$ : 
$$\varepsilon_{ini}^{n+1, tr} = \varepsilon_{p1}^n + \frac{\alpha_2}{c} \left[ (\varepsilon_{p1}^n - \varepsilon_T) + \sqrt{(\varepsilon_{p1}^n - \varepsilon_T)^2 - \frac{2}{\alpha_2} \left( \frac{\alpha_1}{2} (\varepsilon_{p1}^n)^2 - c_T \right)} \right]$$

Loop of n times:

1/predictor step

$$\varepsilon_{eff}^{n+1, tr} = \varepsilon^{n+1} - (1 - \lambda^n) \varepsilon_{p1}^n - \lambda^n \varepsilon_{p2}^n - \lambda^n \varepsilon_T$$

- If  $\varepsilon_{ini}^{n+1, tr} < \varepsilon^{n+1}$  then:

2/ elastic region

$$\varepsilon_{eff}^{n+1} = \varepsilon_{eff}^{n+1, tr}, \lambda^{n+1} = \lambda^n, \varepsilon_{p1}^{n+1} = \varepsilon_{p1}^n, \varepsilon_{p2}^{n+1} = \varepsilon_{p2}^n$$

- If  $\varepsilon_{ini}^{n+1, tr} > \varepsilon^{n+1}$  then:

3/plastic region

$$\varepsilon_{p2, ini}^n = \frac{c}{\alpha_2} (\varepsilon^{n+1} - \varepsilon_{p1}^n) \text{ (Initialize)}$$

$$\varepsilon_{p2}^{n, tr} = \varepsilon_{p2, ini}^n \text{ (ONCE ONLY)}$$

Driving forces:

$$q_1 = c \varepsilon_{eff}^{n+1, tr} - \alpha_1 \varepsilon_{p1}^n$$

$$q_2 = c \varepsilon_{eff}^{n+1, tr} - \alpha_2 \varepsilon_{p2}^n$$

$$q_\lambda = c \varepsilon_{eff}^{n+1, tr} (\varepsilon_{p1}^n - \varepsilon_{p2, ini}^n - \varepsilon_T) - \frac{\alpha_1}{2} (\varepsilon_{p1}^n)^2 + \frac{\alpha_2}{2} (\varepsilon_{p2}^n)^2 + c_T$$

Update internal variables:

$$\lambda^{n+1} = \lambda^n + \Delta t \frac{\eta \gamma}{\eta + \gamma \beta |\varepsilon_{p2}^n - \varepsilon_{p1}^n|} \max \left\{ 0, \left[ c \varepsilon_{eff}^{n+1, tr} (\varepsilon_{p1}^n - \varepsilon_{p2}^n - \varepsilon_T) - \frac{\alpha_1}{2} (\varepsilon_{p1}^n)^2 + \frac{\alpha_2}{2} (\varepsilon_{p2}^n)^2 + c_T \right] - r |\varepsilon_{p2}^n - \varepsilon_{p1}^n| \right\}$$

$$\varepsilon_{p1}^{n+1} = \varepsilon_{p1}^n + \Delta t \cdot \eta \max \left\{ 0, \left[ c \varepsilon_{eff}^{n+1, tr} - \alpha_1 \varepsilon_{p1}^n - r \right] \right\} \text{sign}(q_1^{n+1})$$

$$\varepsilon_{p2}^{n+1} = \varepsilon_{p2}^n + \Delta t \cdot \eta \max \left\{ 0, \left[ c \varepsilon_{eff}^{n+1, tr} - \alpha_2 \varepsilon_{p2}^n \right] - r \right\} \text{sign}(q_2^{n+1})$$

End

$$\text{Stress: } \sigma^{n+1} = \frac{\partial \psi_{mix}}{\partial \varepsilon^{n+1}} = c \cdot \varepsilon_{eff}^{n+1}$$

It is also valuable to make some remarks from the algorithm. First of all, the internal variables will start off being all zeros, as per natural characteristics. Accordingly, these variables will remain unchanged, which are, again, all zeros, throughout the elastic period. The next point is that,  $\varepsilon_{p2}^{n, tr}$  is assigned by the value  $\varepsilon_{p2, ini}^n$  only once at the very beginning of plasticity. As this internal variable evolves, it will be updated via its previous step's value. Also, this element should only be calculated once and not evolving over time. Furthermore, it is essential to assure that the internal variables are only updated when their yield functions, which

are  $\left| c \varepsilon_{eff}^{n+1, tr} (\varepsilon_{p1}^n - \varepsilon_{p2}^n - \varepsilon_T) - \frac{\alpha_1}{2} (\varepsilon_{p1}^n)^2 + \frac{\alpha_2}{2} (\varepsilon_{p2}^n)^2 + c_T \right| - r \left| \varepsilon_{p2}^n - \varepsilon_{p1}^n \right|$ ,  $\left| c \varepsilon_{eff}^{n+1, tr} - \alpha_1 \varepsilon_{p1}^n \right| - r$  and  $\left| c \varepsilon_{eff}^{n+1, tr} - \alpha_2 \varepsilon_{p2}^n \right| - r$ , are non-negative, according to Kuhn-Tucker condition. This assurance might lead to a delay of evolution among these internal variables, which will be depicted in the result and discussion session. Last but not least, the stress is calculated as a derivative of the Helmholtz energy with respect to the overall strain, which results from the Clausius-Duhem Inequality applied on temperature independent system, which the material being studied represents. The derivative ends up giving a very satisfying, comfortable-to-compute equation of stress:

$$\sigma^{n+1} = c \cdot \varepsilon_{eff}^{n+1}, \quad (28)$$

The handy algorithm mentioned above is then applied on MATLAB, as the programme provides a matrix-friendly environment, which is very attractive in terms of calculation involving arrays or matrices.

#### 4. Result and discussion

With the aid of the algorithm, calculation of the internal variables as well as material response can be immediately executed. We would like to focus on how the response curve (i.e stress-strain curve), the two plastic strains, and the volume fraction reacts to different values of each material parameter, which are the hardening parameters  $\alpha_1$ ,  $\alpha_2$ , and  $\beta$ , the viscous parameters  $\eta$  and  $\gamma$ , the evolution threshold  $r$ , and the phase transformation parameters  $\varepsilon_T$  and  $c_T$ . Chosen values of the parameters to company with the investigations are given as following, unless the parameter is under investigation:

$$c = 1.5;$$

$$\eta = 0.002;$$

$$c_T = 0.004;$$

$$r = 0.001;$$

$$\varepsilon_T = 0.05;$$

$$\gamma = 4;$$

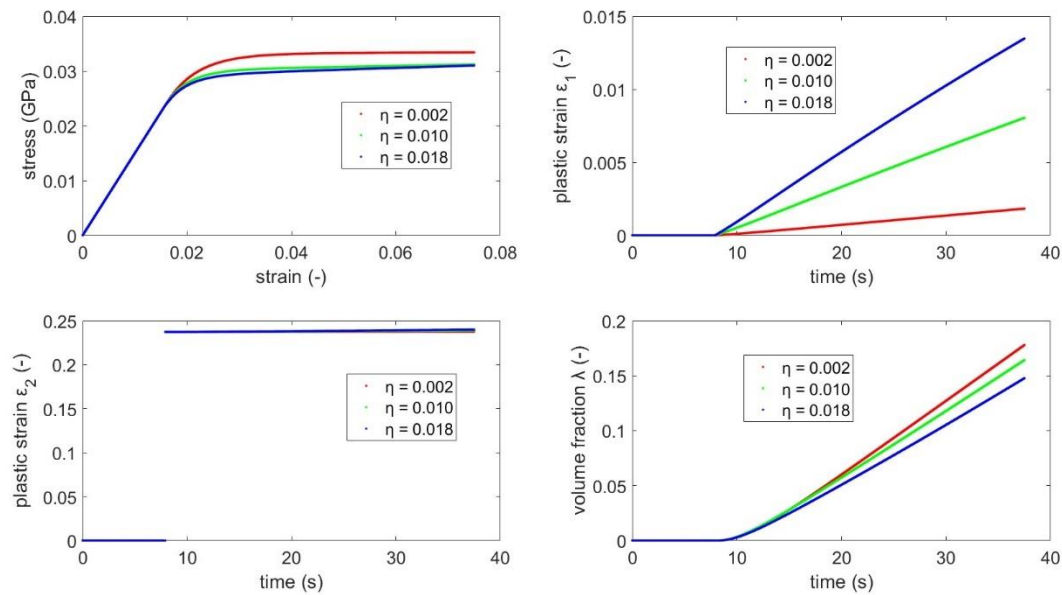
$$\beta = 0.001;$$

$$\alpha_1 = 0.5;$$

$$\alpha_2 = 0.1;$$



The influence of viscous parameter  $\eta$  on aforementioned aspects is first to be examined. Fig.1 illustrates the how material behaves under different values of  $\eta$ .



**Fig. 1** Material behaviour under several tested values of viscous parameter  $\eta$ . Depicted are the stress-strain curve, the evolution of  $\varepsilon_{p1}$  and  $\varepsilon_{p2}$  respectively, as well as second-phase volume fraction.

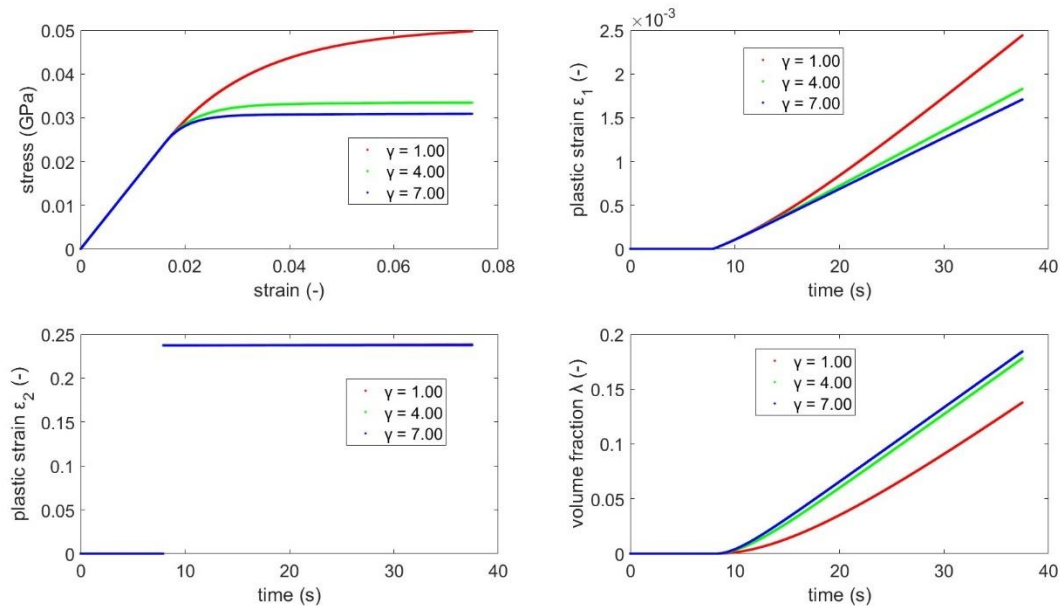


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It is obvious that this viscous parameter plays an important role on the evolution of plastic strain  $\varepsilon_{p1}$ , as higher values of  $\eta$  results in a faster rate of growth of  $\varepsilon_{p1}$ , which simultaneously means a higher yielded value of this plastic strain at each time step. This behaviour can also be observed from the second-phase plastic strain  $\varepsilon_{p2}$ , however the effect is very diminutive compared to that of  $\varepsilon_{p1}$ . On the other hand,  $\eta$ 's increase brings about a lower pace of growth of the volume fraction  $\lambda$ , thus lower values at the same time step. Even more so, though hard to be monitored on graphs, it is still obvious from data sheet that the higher the value of  $\eta$ , the more it delays the evolution of volume fraction  $\lambda$ . Last but not least, the increase of  $\eta$  also results in lower response.

Another viscous parameter being under investigation is  $\gamma$ . Though also being a viscous parameter, the influence of different  $\gamma$  on the material might show some discrepancies compared to that by differing  $\eta$ . First of all, increasing  $\gamma$  and increasing  $\eta$  influence the plastic strain  $\varepsilon_{p1}$  and the second-phase volume fraction  $\lambda$  in opposite manner. As shown in

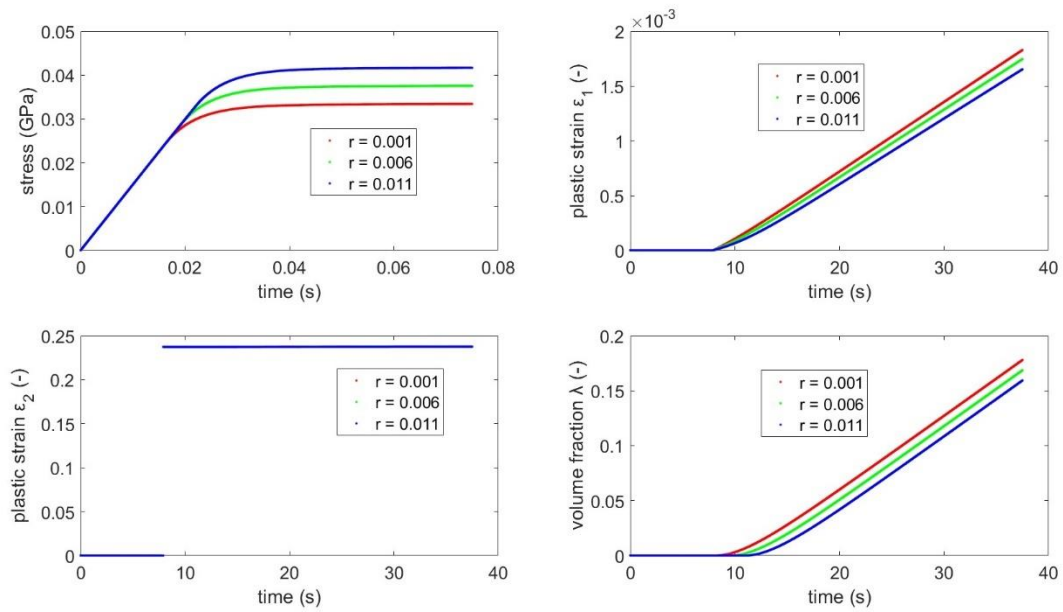
Fig. 2b and Fig. 2d, enlarging  $\gamma$  causes lower growth of  $\varepsilon_{p1}$ , but higher values of volume fraction  $\lambda$ .



**Fig. 2** Material behaviour under different values of viscous parameter  $\gamma$ . The order of images is equivalent to that of **Fig. 1**

It is also note-worthy that, this viscous parameter influences the rate of change of  $\varepsilon_{p1}$  in a more subtle manner, which is illustrated in Fig. 2b. However, interestingly, in contrast with  $\eta$ , the viscous parameter  $\gamma$  does not beget any delay in the evolution of plastic strain. The very minute difference of  $\varepsilon_{p2}$ 's response according to different  $\gamma$  is also obvious from Fig. 2c. What is more, the volume fraction  $\lambda$  yields at later time step compared to  $\varepsilon_{p1}$  and  $\varepsilon_{p2}$ . Besides, increasing  $\gamma$  causes the response curve to drop heavily in terms of value. Last but not least, though gamma is increased in a very drastic manner, the difference in material response results from the second jump of gamma in terms of value is not very distinguished compared to that of the first increase of gamma. This behaviour might anticipate a “reduced” influence on material response regarding raising gamma.

We further investigate how changing evolution threshold  $r$  might affect the material. The reaction of the response curve, the plastic strains and the volume fraction are displayed below.



**Fig. 3** Influence of changing evolution threshold  $r$

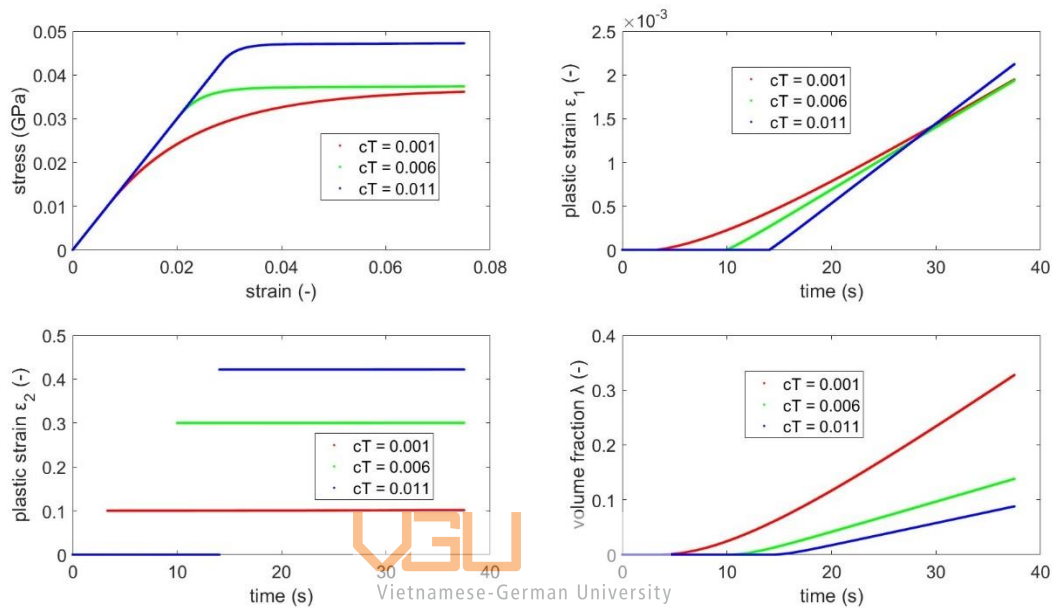
First of all, the volume fraction's reaction to the change of the evolution threshold depicted in the graph shows some agreement with its evolution equation. Equation (22) shows clearly that the yield function might turn negative if we increase the value of  $r$ . Accordingly, this will apparently delay the evolution of the second-phase volume fraction. Indeed, this delay is well-illustrated in Fig. 3d. What is more, interestingly, as its name would suggest, the evolution threshold  $r$  would raise the yield strength of the material as it increases. Another aspect is that, once again, this parameter has almost no influence on second-phase plastic strain  $\varepsilon_{p2}$  as we make modification to its value.

There are two parameters that might play a significant role in material behaviour, which appear to be the transformation parameter  $c_T$  and transformation strain  $\varepsilon_T$ . The significance might come from the fact that they represent the phase transformation of the material, as well as the requirement of them being much smaller than the material's elastic moduli:

$$\frac{c_T}{\varepsilon_T} \ll c, \quad (29)$$

As a result, while investigating one of the two parameters, it is worth mentioning the chosen value of the other.

We might start with the analysis of transformation parameter  $c_T$ . The transformation strain  $\varepsilon_T$  of 0.05 is chosen to pair with the following sets of  $c_T$  in order to keep the system under the condition (29). The calculated responses of the material are displayed in Fig. 4:

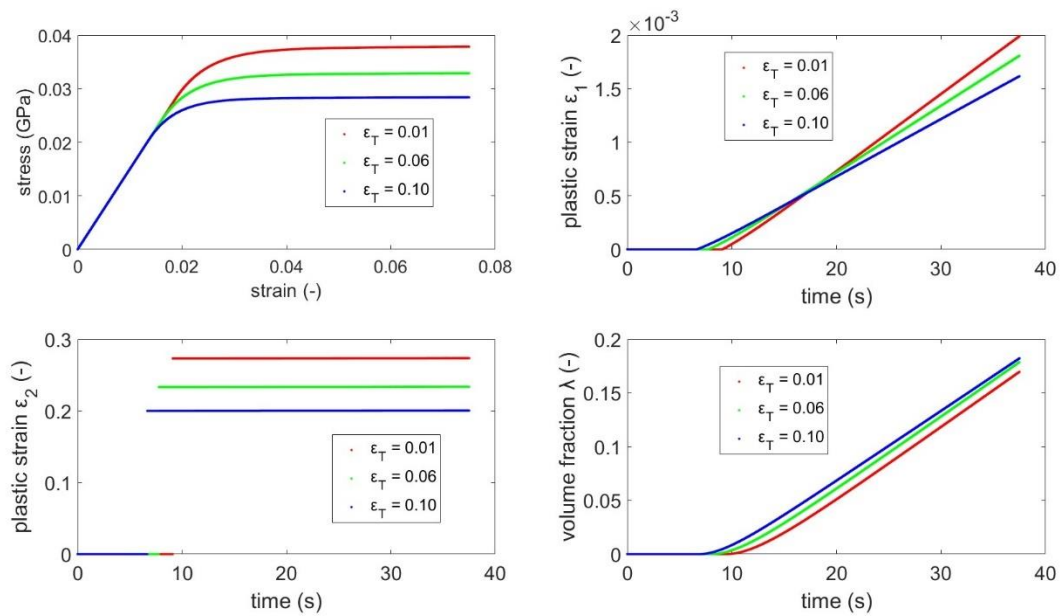


**Fig. 4** Different material behaviour with respect to change of  $c_T$ , paired with  $\varepsilon_T = 0.05$

It is apparent from Fig. 4 that, changing  $c_T$  alters all of the aspect of the material behaviour. Increasing  $c_T$  not only delays the evolution of microstructure, but also the evolution of all internal variables. Undoubtedly, this is due to the fact that,  $c_T$  has a direct influence on the microstructure-initiating value of the overall strain  $\varepsilon$ , given in equation (27). Subsequently, the higher  $c_T$  is, the higher  $\varepsilon_{ini}$  and therefore  $\varepsilon^{n+1}$  is, which results in latency in this evolution of  $\varepsilon_{p2}$ . It can also be clearly seen from the figure above that, higher values of  $c_T$  engender higher values of resultant stress and second-phase plastic strain  $\varepsilon_{p2}$ . On the other hand, raising  $c_T$  significantly softens the growth of first-phase plastic strain  $\varepsilon_{p1}$  and volume fraction  $\lambda$ .

On the other hand, the rise of the transformation strain  $\varepsilon_T$  brings about an absolute opposite influence on the material compared to increasing  $c_T$ . Clear results of the investigation

can be found in Fig. 5. Note that  $c_T$  is assigned the value of 0.004 GPa in this investigation of different  $\varepsilon_T$ .

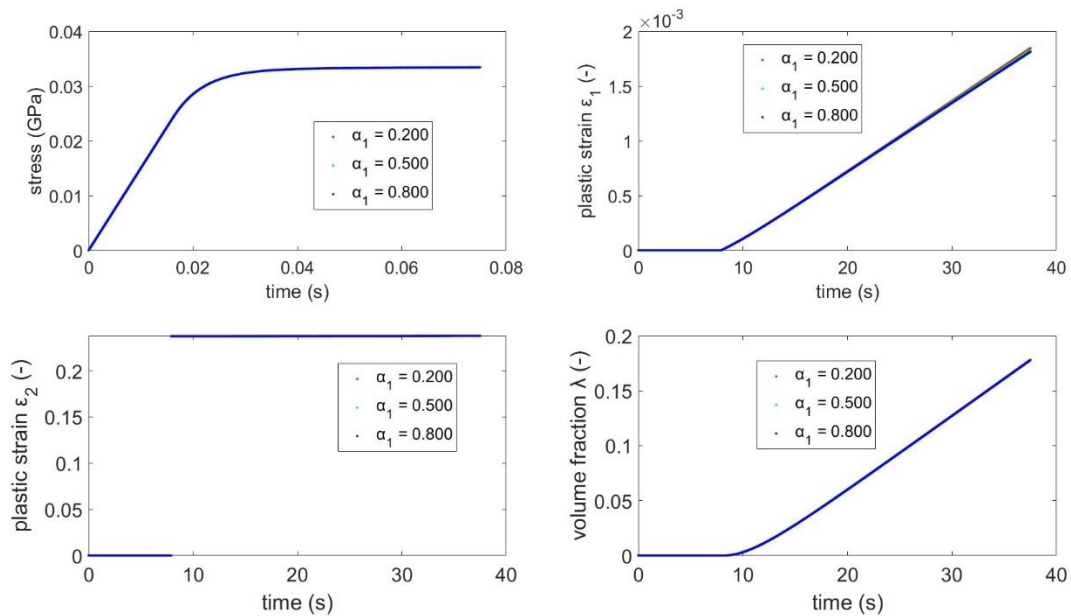


**Fig. 5** Influence of transformation strain  $\varepsilon_T$  on material behaviour

Unsurprisingly, this phenomenon can be anticipated from evolution equations and stress equation. There,  $\varepsilon_T$  appears to carry a negative (-) sign, as opposed to  $c_T$ . As a result, raising  $\varepsilon_T$  is actually lowering down the eventual values of the internal variables and the stress itself. Furthermore, changing  $\varepsilon_T$  does also alter the yielding time of the internal variables, as can be observed in image 2b, 2c and 2d.

We are also fond of examining the influence of the hardening parameters on the material. However, a small remark should be declared, that is, as a matter of fact, the hardening parameters should always be much smaller than the elastic moduli itself. In this specific case, we also chose the parameters under a condition that:

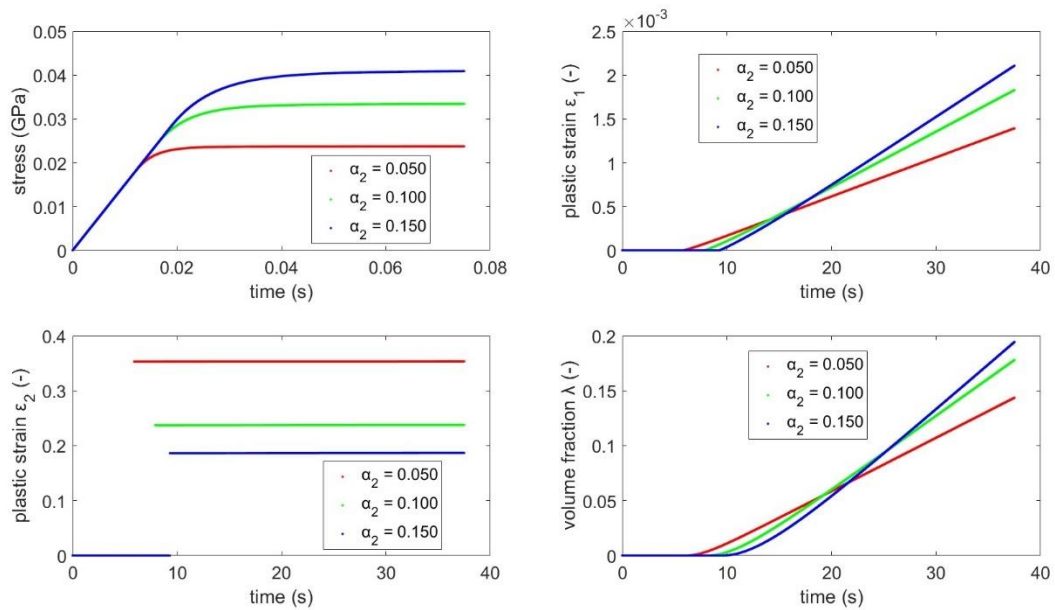
$$\alpha_1 > \alpha_2$$



**Fig. 6** Influence of hardening parameter  $\alpha_1$  on the material

Chosen value of  $\alpha_2$  to be paired with the set of  $\alpha_1$  is 0.1 GPa. Intriguingly, as illustrated in Fig. 6, altering the hardening parameter  $\alpha_1$  brings about almost no clear discrepancy in material behaviour.

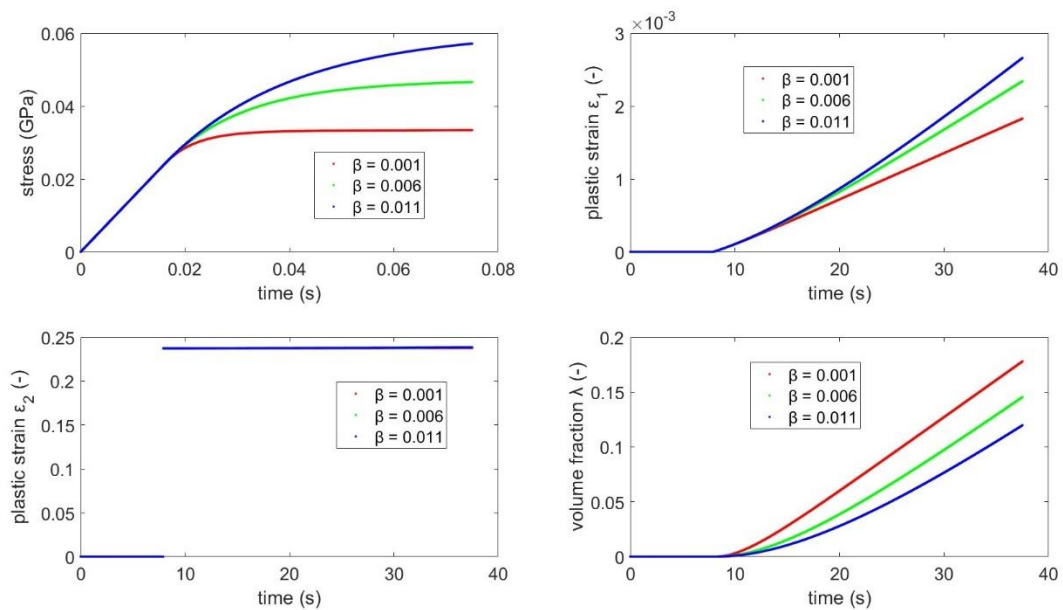
However, in contrast, the material does react differently while changing the hardening parameter  $\alpha_2$ . As pictured in Fig. 7, increasing  $\alpha_2$  not only changes the moment of yielding of the internal variables, but also their pace of growth. Specifically, increasing  $\alpha_2$  results in higher ultimate yield strength of the material, which would be very appealing as the material would be able to handle more load. What is more, further increasing  $\alpha_2$  causes plastic strain  $\epsilon_{p1}$  and volume fraction  $\lambda$  to yield later but with faster pace. However, this effect is flipped over in terms of second-phase plastic strain  $\epsilon_{p2}$ .



**Fig. 7** Material reaction in regard to altering hardening material  $\alpha_2$ , paired with  $\alpha_1 = 0.5 \text{ GPa}$



The very final material that we would examine is the hardening parameter  $\beta$ . Illustrated in Fig. 8 below is the material behaviour in regard to altering this hardening parameter.



**Fig. 8** Different material response regarding altering hardening parameter  $\beta$

First of all, the result shows a contravariant manner between  $\beta$  and volume fraction  $\lambda$ . In other words, increasing  $\beta$  begets a decrease in both pace of growth and value of the volume fraction. Furthermore, higher value of  $\beta$  also results in higher ultimate yield strength, which is rather appealing. Once again, altering  $\beta$  has the slightest of influence on second-phase plastic strain  $\varepsilon_{p2}$ . This might be explained by the fact that hardening parameter  $\beta$  does not appear directly in the evolution equation of  $\varepsilon_{p2}$ .

## 5. Conclusion

Firstly, we have introduced the theoretical basis for this particular problem, which is a one-dimensional problem of an elasto-viscoplastic material with isotropic hardening. Then we have proposed a suitable algorithm in order to compute the evolutions equations that come along with the theoretical basis, which eventually give the values of the stress, as well as all the mentioned internal variables. Using the algorithm, we further investigated the influence of material parameters on the material itself. To sum up, most of the increase of parameters would affect the yielding time of the internal variables, as well as their pace of growth, which can be observed as their curves having different slopes according to different parameter values. What is more, changing the parameters will finally alter the response curve, which actually means different ultimate yield strength for different parameter values. Interestingly, some changes of behaviour by differing the parameters can be anticipated by the given equations from the theory. Finally, it is very appealing to have further investigation on the cross effect of the parameters on the parameter behaviour, which requires changing several parameters at once.

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