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# Optimization-based procedure for the determination of the constitutive model coefficients used in machining simulations

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## Abstract

This paper deals with the determination of the constitutive model coefficients used in machining simulations. An optimization-based procedure is developed and applied to constitutive model coefficients determination of Ti6Al4V titanium alloy. The procedure is implemented in LS-Dyna/LS-Opt software, coupled with Abaqus/Explicit to calculate the force-displacement curve at each iteration, which is required for the optimization-based procedure. The robustness of the procedure to determine the constitutive model coefficients is evaluated by comparing the predicted and measured plastic strain distributions in the samples.

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**Keywords:** Modelling; Machining; Constitutive model

## 1. Introduction

As a difficult-to-machine material, Ti6Al4V titanium alloy induces short tool life and poor surface integrity. Numerical simulation of machining is an effective method to predict those outcomes without performing time consuming and expensive machining tests. Moreover, the constitutive model, which describes the mechanical behaviour of the work material, is crucial for the simulations.

Johnson-cook (JC) constitutive model [1] is available in almost the commercial finite element method (FEM) software and often used in numerical simulations of several process, including: high velocity impact, metal forging and machining. This model considers the strain hardening, strain rate and temperature effects on the material plasticity and damage. However, it lacks to reproduce the state of stress effects in the

material plasticity and damage. Bai and Wierzbicki [2] introduced a constitutive model by accounting for the state of stress, which is characterized by two parameters: the stress triaxiality  $\eta$  and the Lode angle ( $\bar{\theta}$ ). The stress triaxiality ( $\eta$ ) is a ratio of mean stress  $\sigma_m$  and the equivalent von-Mises stress. The Lode angle ( $\bar{\theta}$ ) is defined by the angle between the stress tensor that passes through the deviatoric plane and the axis of the principal stresses [2].

The determination of the constitutive model coefficients is an important task in the model setup. The goal is the determination of the coefficients values for a give material based on experimental data, mainly coming from mechanical tests. Melkote et al. [3] present different methods, including direct and inverse methods, which can be used to determine the constitutive model coefficients. The inverse methods based on optimization algorithms are appropriate for determining the

coefficients of complex constitutive models involving many variables. The inverse method consists of simulating the experimental test by modifying the constitutive model parameters iteratively to minimize the difference between the predicted and measured data. As mentioned by Melkote et al. [3], several optimization algorithms can be used for this purpose, organised in three main groups: gradient-based, derivative-free search and evolutionary algorithms. Depending on the applied determination method, different constitutive model coefficients can be generated. So, this may contribute to the dispersion of coefficients values found in the literature for the same material, as it is the case of the JC model of Ti6Al4V titanium alloy [4-6].

In this paper, an optimization-based procedure is proposed to determine the constitutive model coefficients of Ti6Al4V titanium alloy. To determine the model coefficients, different specimens and tests configurations are designed and the corresponding mechanical tests are performed. Then, based on the experimental data from these mechanical tests, the coefficients are determined using the optimization-based method implemented in LS-DYNA/LS-Opt software.

## 2. Constitutive model

Cheng et al. [8] proposed a constitutive model to describe the mechanical behavior of Ti6Al4V alloy in metal cutting, which includes the strain hardening, strain rate and state of stress effects. Since the plasticity (flow stress) is the most important part of this model, it is used in this study to demonstrate the determination of the constitutive model coefficients, considering the optimization-based procedure. This plasticity part of the constitutive model is given by the following equation:

$$\bar{\sigma} = [A + m\epsilon_p^n] [B + C \ln(E + \frac{\dot{\epsilon}}{\dot{\epsilon}_0})] [1 - c_\eta(\eta - \eta_0)] [c_\theta^s + (c_\theta^{ax} - c_\theta^s) (\gamma - \frac{\gamma^{a+1}}{a+1})] \quad (1)$$

where: i)  $A$ ,  $m$ , and  $n$  are material coefficients for strain hardening effect; ii)  $B$ ,  $C$ ,  $E$  are the material coefficients for strain rate effect; iii)  $c_\eta$  is a material coefficient for stress triaxiality effect; iv)  $c_\theta^t$ ,  $c_\theta^c$ ,  $c_\theta^s$ , and  $\alpha$  are the material coefficients for the Lode angle effect; v)  $\eta_0$  and  $\dot{\epsilon}_0$  are the reference stress triaxiality and reference strain-rate, respectively; vi) the coefficient  $\gamma$  represents the difference between von-Mises and Tresca equivalent stresses in the deviatoric stress plane; and vii) the coefficients  $c_\theta^t$ ,  $c_\theta^c$ ,  $c_\theta^s$  are correlated and at least one of them equals to one [2]. For example, in compression test of cylindrical specimens at quasi-static conditions,  $\eta_0$  is  $-1/3$ ,  $\dot{\epsilon}_0$  is  $0.05 \text{ s}^{-1}$  and  $c_\theta^c$  is 1.

The temperature effect isn't considered in this plasticity model for two main reasons. First, commonly mechanical tests at high strain rates already include the effect of temperature on the mechanical behaviour. Second, the temperature of the workpiece in the primary deformation zone in metal cutting hardly exceeds  $200^\circ\text{C}$  due to mass transportation (i.e. heat advection) by the moving chip [7,8].

## 3. Specimen geometries and mechanical tests

According to the constitutive model, 13 coefficients

associated to three factors affecting the mechanical behaviour (strain hardening, strain rate and state of stress effects) need to be determined. For this reason, different specimens' geometries are designed and fabricated, to generate a wide range of stress-states [8]. Therefore, five specimens' geometries are selected for the mechanical tests: cylindrical, smooth round bar (SRB), notched round bar (NRB), double notched (DN) specimen and notched flat plate (NFP). Then, tensile and compression tests at quasi-static conditions and at different strain rate were performed. Quasi-static (compression and tensile) tests of all above-mentioned specimen's geometries were performed at room temperature on the servohydraulic machine (Fig. 1). This machine is equipped with a Digital image correlation (DIC) system composed by two CCD cameras and DIC software, to determine the displacement and strain distribution at the specimen's surface [9]. An extensometer is also used to measure the local displacement between two gauge points.

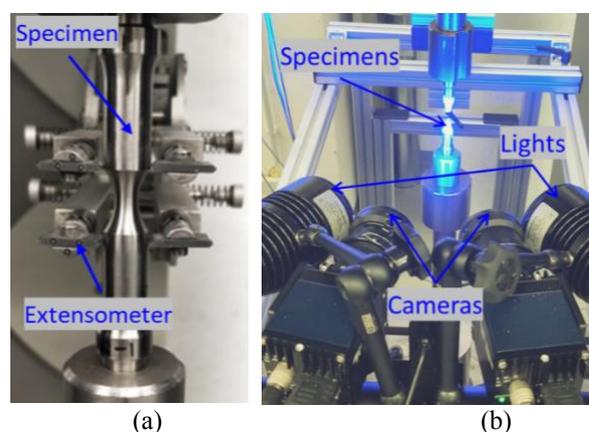


Fig. 1. Tensile test of a round bar on a servohydraulic machine equipped with: a) extensometer; b) 3D DIC system.

As an example, Fig. 2 shows the force-displacement curves obtained from the tensile tests of SRB. However, to determine the constitutive model coefficients the force-displacement curves were also obtained for the other specimens' geometries.

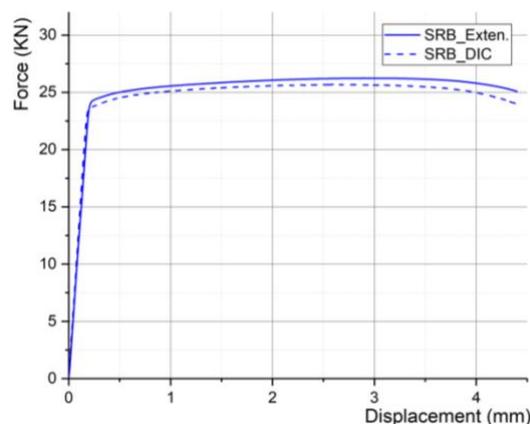


Fig. 2. Force – displacement curves of tensile tests of SRB using both 3D DIC and extensometer

Furthermore, a Split Hopkinson Pressure Bar (SHPB) apparatus was used to perform the compression tests of cylindrical specimens at different strain rates.

#### 4. Determination of the constitutive model coefficients

##### 4.1. Procedure description

To determine the constitutive model coefficients, four combinations mechanical tests and specimens' geometries are used. The first combination is the compression test using cylindrical specimen, which are used to determine the coefficients related to the strain hardening and strain rate ( $A, B, C, m, n$  and  $E$ ). Since, the reference test is defined as the quasi-static compression tests of cylindrical specimens, the reference coefficients are given by:  $\eta_0 = -0.333$ ,  $\dot{\epsilon}_0 = 0.05 \text{ s}^{-1}$  and  $c_\theta^c = 1$ . The second combination is the compression test using double notched specimen, used to determine the  $c_\eta$  and  $c_\theta^s$  coefficients. The third combination is the tensile test using notched round bar, which are used to determine the remaining coefficients,  $c_\theta^t$  and  $a$ .

The coefficients are determined using the following sequential steps: 1<sup>st</sup>)  $A, B, C, m, n$  and  $E$  coefficients; 2<sup>nd</sup>)  $c_\eta$  and  $c_\theta^s$  coefficients; and 3<sup>rd</sup>)  $c_\theta^t$  and  $a$  coefficients. In each step, some initial model coefficients are determined using a direct method, based on the nonlinear least square method. Then, these coefficients are used as initial values in an optimization-based procedure to determine their optimal ones. As shown in Fig. 3, this procedure consists into simulate the experimental test by modifying the constitutive model parameters iteratively to minimize the difference between the predicted and experimental measured force-displacement curves. At each iteration a new set of coefficients are calculated by an optimization-based procedure. This procedure is implemented in LS-Opt software, an optimization software module from LS-Dyna. This software can be connected to FEA software to run the numerical simulations, such as Abaqus/explicit, used in this work.

Fig. 4 shows the implementation of the optimization-based

procedure in Ls-Opt software. This figure shows the particular case of the determination of the strain hardening and strain rate coefficients ( $A, B, C, m, n$  and  $E$ ) of the plasticity model. The procedure is composed by the following steps: 1) coefficients initialisation (initial values); 2) selection of the best coefficients values from a given range, using a Design of Experiments (DoE) method; 3) run mechanical tests simulations in Abaqus/Explicit; 4) build metamodel; 5) comparison between calculated and measured force-displacement curves, applying Curve Mapping Segment (CMS) or Mean Squared Error (MSE) methods; 6) execute metamodel optimization using hybrid adaptive simulated annealing (ASA) and Leapfrog Optimizer for Constrained Minimization (LFOP) algorithms; and 7) verification of the termination criterion.

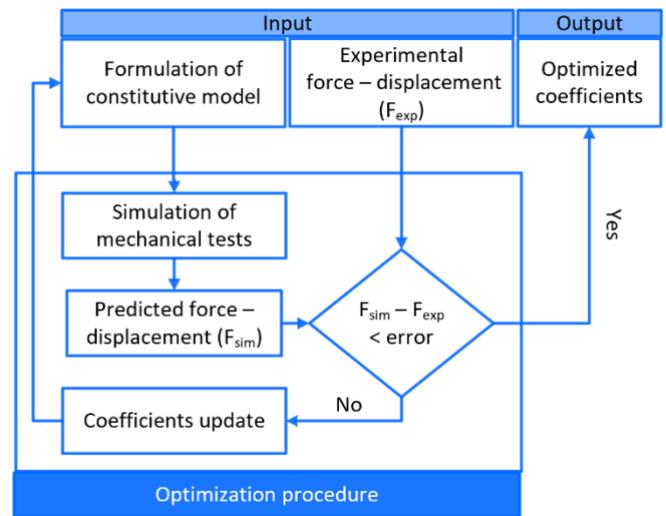


Fig. 3. Flowchart of the optimization-based procedure

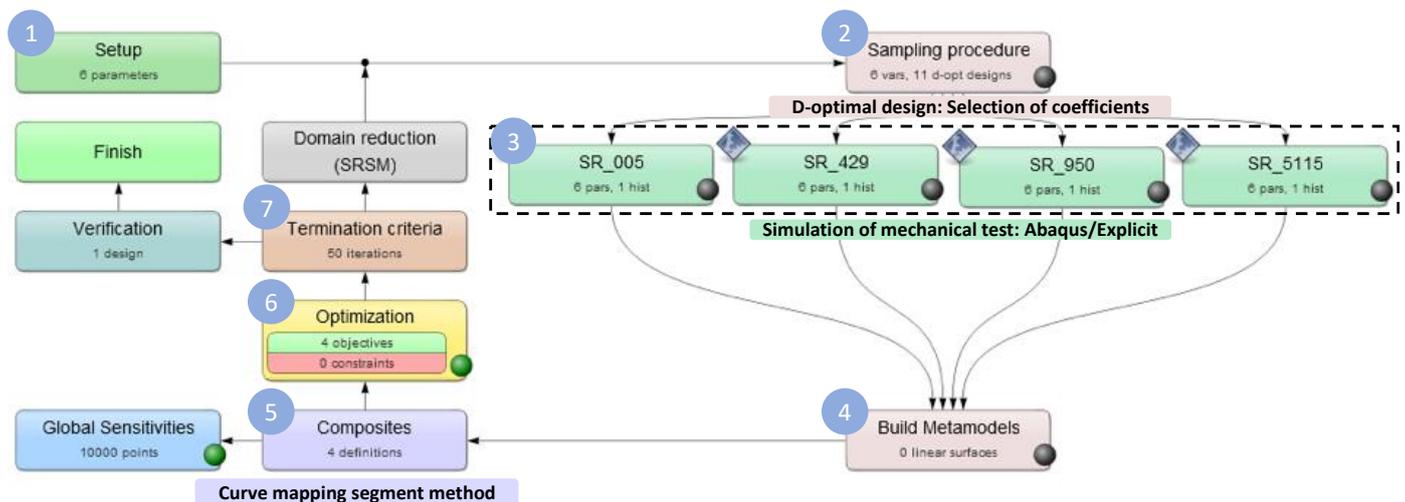


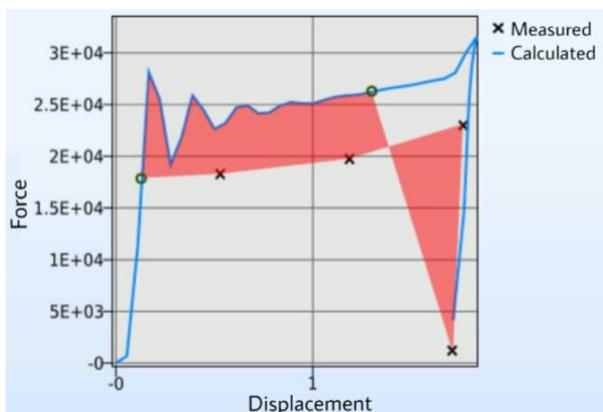
Fig. 4. Optimization-based procedure of the model coefficients determination using the compression tests of cylindrical specimens in Ls-Opt software.

Since the quasi-static compression test of a cylindrical specimen is the reference test, Eq. 1 is reduced to the first two terms, i.e., the strain hardening and strain rate terms. The initial coefficients values and corresponding ranges are determined using the results from the cylindrical specimens by applying a direct method [3]. Then, a DoE method (D-optimal design) is

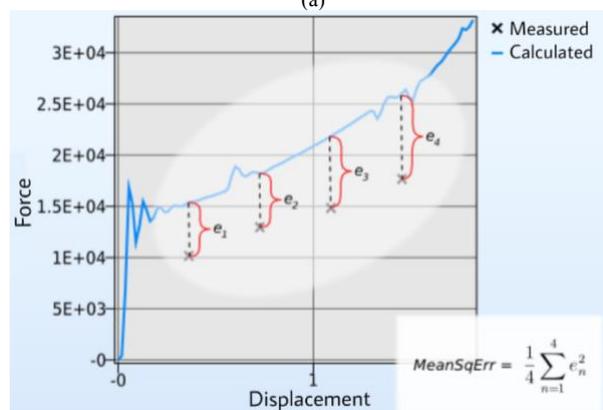
applied to select the best (optimal) set of coefficients values to build a response surface. For small number of coefficients, the full factorial design is used, otherwise a space filling method is applied [10]. Therefore, a good balance between accuracy and computational time can be achieved.

After the coefficients values have been selected, Abaqus/explicit is used to simulate the compression test of the cylindrical specimens at different strain rates. Then, the obtained calculated force-displacement curves are exported to LS-Opt software and compared with the experimental measured ones. To evaluate the difference between them, the CMS method is used, which calculates the smallest area between the measured and calculated force-displacement curves (Fig. 5a). In this method, a segment with the same length as the measured curve is moving from the starting point to the end point of the calculated curve, until the smallest polygon between this segment and measured curve is found [11]. Additionally, the MSE method calculates the sum of the squares of the distances in the y-coordinate between the target points and the interpolated points on the calculated curve (Fig. 5b). Compared with the MSE method, the CMS method incorporates both the ordinate and the abscissa into the difference computation, so the hysteric curve and vertical sections of curve can be identified [11].

In the next step of optimisation-based procedure, the difference between the calculated and the measured force-displacement curves is minimized using a hybrid algorithm, which uses ASA algorithm to find an approximate global optimum solution, followed by LFOP algorithm to sharpen this solution.



(a)



(b)

Fig. 5. Difference between calculated and measured force-displacement curves evaluated by a) MSE method; b) CMS method [11].

After each iteration a termination criterion (force-displacement error and maximum number of iterations) is checked and if it is not satisfied the sequential response surface (SRS) method is applied to build a new response surface for the

next iteration. The typical feature of this method is that the size of the subregion (range of determined coefficients) is adjusted at each iteration, which gives higher accuracy when optimizing using metamodels. The optimization process stops when the termination criterion is satisfied. The above-described optimisation-based procedure was also applied to determine other constitutive model coefficients.

#### 4.2. Verification

In order to evaluate the robustness of the proposed optimisation-based procedure to determine the constitutive model coefficients, predicted and measured plastic strain distributions in the deformed samples are compared. The predicted plastic strain distribution was obtained by numerical simulation of the mechanical tests, while the measured one was obtained from the mechanical tests using the DIC technique. This analysis was performed on samples not used in the coefficients' determination procedure.

Fig. 6 shows the equivalent plastic strain distribution measured by DIC technique (right side) and that predicted by the numerical simulation (left side) of the compression test of the DN specimens with pressure angle 60°.

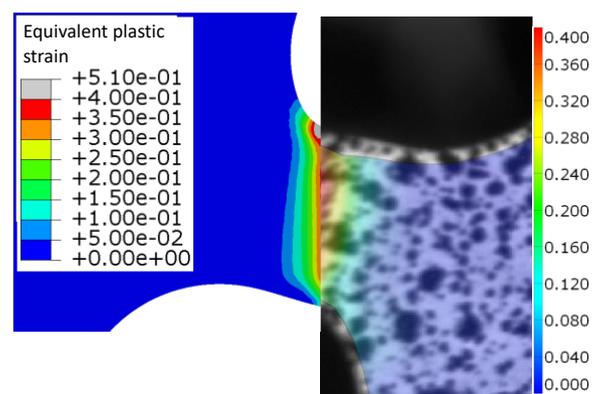


Fig. 6. Equivalent plastic strain distribution in the DN specimen (pressure angle of 60°) at damage initiation, obtained by numerical simulation (left side) and measured by DIC (right side).

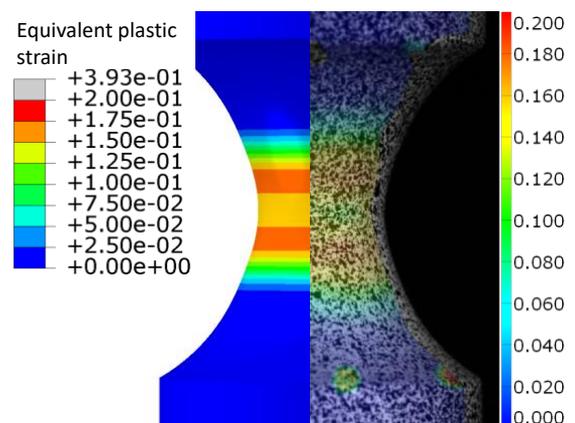


Fig. 7. Equivalent plastic strain distribution in the NRB (notch radius of 6 mm) at damage initiation, obtained by numerical simulation (left side) and measured by DIC (right side).

These strain distributions are obtained at damage initiation, when the strength of workpiece starts to degrade. This figure shows that the measured and predicted plastic strain distributions are identical, showing a plastic strain localization

in the centre of the specimen. Identical numerical simulation was performed for the NRB with a notch radius of 6 mm. Fig. 7, shows the equivalent plastic strain distribution in this sample, obtained by simulation (left side) and measured by DIC (right side). As can be seen by this figure, these equivalent plastic strain distributions are identical.

## 5. Conclusions and outlook

An optimization-based procedure was successfully applied to determine the constitutive model coefficients of Ti6Al4V titanium alloy. This procedure was implemented in LS-Opt optimisation software, connected with Abaqus/explicit for the numerical simulations.

A comparison between predicted and measured plastic strain distributions in the deformed samples has demonstrated the robustness of the proposed optimisation-based procedure to determine the constitutive model coefficients.

As outlook, the determined constitutive model coefficients will be used in a machining model of Ti6Al4V, to predict the machined surface integrity.

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