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SENSITIVITY ANALYSIS OF THE CELLULAR AUTOMATA FINITE ELEMENT MODEL FOR THE STRAIN LOCALIZATION

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Abstract

Application of the sensitivity analysis methods to identify the influence of the multi scale Cellular Automata Finite Element model parameters on the model response is the subject of this work. The sensitivity analysis is based on the Morris method. Description of the basic principles of this method is presented in the paper. Advantages and disadvantages of this approach are discussed, as well. Finally, obtained results of the sensitivity analysis are presented and their importance for further inverse analysis is highlighted.

Key words: multiscale modelling, CAFE model, sensitivity analysis, screening methods, Morris design

1. INTRODUCTION

Accuracy of simulations of materials processing depends on quality of the description of phenomena occurring during deformation. Rheological models usually treat material as a continuum and are unable to describe properly several important phenomena, which may be either random or discontinuous or even both. Therefore, there is a continuous search for alternative models, which account for non-continuous structure of materials and for the fact, that various phenomena in the materials occur in various scales. Accounting for the stochastic character of phenomena is an additional challenge. Multiscale models, see e.g. [1], are one of the solutions capable to overcome mentioned difficulties.

Authors have developed multiscale models based on combination of the Finite Element (FE) and Cellular Automata (CA) methods. Such model is designed to describe development of the strain localization during materials processing [2]. Numerical tests confirmed qualitatively good predictive capability of the model. Problem of quantitative accuracy still remains open. To reach this accuracy, the values of the coefficients in the transition rules of the CAFE model have to be determined on the basis of the experimental data. It is expected that inverse analysis should be an efficient method to identify these parameters [3]. Since this analysis is usually very costly, it should be preceded by the sensitivity analysis and selection of the parameters, which are of particular importance. Thus, the objectives of the present work is to perform the sensitivity analysis to identify key parameters of the model and to determine their influence on the model response. Numerical simulation of the simple shearing tests is used as a case study.

2. CAFE MODEL

The CAFE model is a multi scale approach, which accounts for phenomena that occur at different scales in the material. Initiation and development of the micro and macro shear bands during various

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forming processes is one of the examples of such phenomena. Micro shear bands initiate and propagate in the microscale, while shear bands appear at the mezoscale. According to these two scales, two cellular automata spaces that represent material behaviour in the micro- and mezoscale are introduced and attached to the commercial Forge2 FE code.

In the CAFE model both CA spaces, micro shear band space (MSB space) and shear band space (SB space), are defined by several state variables that describe each particular cell, as well as by a set of transition rules defined respectively for those spaces. Transition rules provide an information when a CA cell can change its state and become a cell with micro shear bands (*activeMSB*) or shear bands (*activeSB*) in the MSB and SB space, respectively. Transition rules are usually logical functions, which are used to replicate mechanisms leading to initiation of micro shear bands and shear bands that are observed experimentally [4,5]. When the transition rules are fulfilled particular cell can change its state i.e. to state *activeMSB* if not the state of the cell remain unchanged. Detailed description of the developed model regarding state of the cells and transition rules is presented in other authors works [6,7].

Information about the occurrence of micro shear and shear bands is exchanged between the CA spaces during each time step, according to the defined mapping operations. Flow of the information between the scales is performed in both directions, from macroscale to mezoscale and microscale as well as from microscale and mezoscale to macroscale. In each time increment, information about stress tensor is sent from the finite element solver to the MSB space, where development of micro shear bands is calculated according to the transition rules. After exchange of information between CA spaces, transition rules for the SB space are introduced, and propagation of shear bands is modelled. Based on the information supplied by the CA spaces, the flow stress σ_p^{CA} is calculated and is used in the FE program during the next step of the FE calculations.

Gauss function is used in the model to control distribution among the cells of one of the internal variables for the MSB space. A critical value for initiation of the hard slip system, $\tau^*_{\max}$, is the controlled variable described by:

$$\tau^*_{\max} = \frac{1}{\sigma_{dev}\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma_{dev}^2}\right) \tag{1}$$

where: x – expected value, σ_{dev} – standard deviation.

This work is focused on validation of the CA model, in particular, on verification which parameters of the model are of importance in forming of micro shear and shear bands.

Two parameters of the Gauss distribution function are considered as independent stochastic variables in the analysis. One is the expected value x and the standard deviation σ_{dev} is the second one. Values of $\tau^*_{\max}$ are generated using right hand side of equation (1) and they are the main parameters (figure 1), which control the initiation of the micro shear bands in the MSB space according to the transition rule:

$$\mathrm{Y}_{m(MSB)}(t_{i+1}) = \begin{cases} activeMSB & if \quad A \\ \mathrm{Y}_{m(MSB)}(t_i) & otherwise \end{cases}$$

where
$$A = \left(\sigma > \tau^*_{\max}\right) \vee \begin{pmatrix} \mathrm{Y}^m_{l(MSB)} = activeMSB \wedge \\ \theta_m^{rot} - \theta_l^{rot} > \theta \end{pmatrix} \tag{2}$$

where: $\mathrm{Y}_{m(MSB)}(t_{i+1})$ – state of the m^{th} cell from the MSB space at the t_{i+1} time step, *activeMSB* – state of the cell with micro shear bands, σ - stress value obtained form the FE program, $\mathrm{Y}^m_{l(MSB)}$ - state of the l^{th} neighbour of the m^{th} cell from the MSB space, θ - rotation angle.

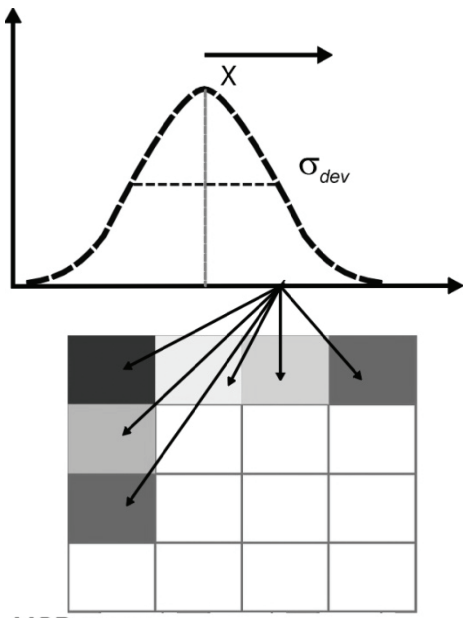


Fig. 1. *Illustration of the $\tau^*_{\max}$ generation using right hand side of the Gauss distribution function, degree of the grey colour indicates different values of this coefficient.*

Other parameters in the transition rules are more related to the propagation of already initiated bands, and at this stage they are not a subject of the investigation.

The third parameter that is taken into account during the analysis is the friction coefficient. Finally the screening sensitivity analysis method [8] is applied here to evaluate importance of the mentioned parameters.

3. MORRIS OAT DESIGN

The Morris design belongs to the class of screening methods [8]. Screening designs, as a part of the sensitivity analysis methods [9], deal with the question which factors of the physical model or computer simulation are really important. The factor means either parameter, which describes properties of the model or input variable, which is directly observable in the corresponding real system. Screening methods estimate qualitative statistic of the factors in order of their importance, i.e. they state that one factor is more important than another, but they do not provide the quantitative information of the factors significance. Screening designs widely use the One-At-a-Time (OAT) approach. Methods based on the OAT technique investigate the impact of the variation of each factor in turn. The OAT design developed by Morris [10] is called the global sensitivity analysis, because the algorithm explores the entire space over which the factors vary. In this algorithm the main effect of the factor is estimated by computing the assumed number of local measures at different points in the input space and next the average value is taken. These points are selected in such a way that each factor covers the whole interval in which it was defined. The key definitions and steps of Morris design are presented below.

Assumptions and definitions. Let **x** is the k-dimensional vector of simulation factors x_i. The components x_i, $i = 1 \dots k$, accept p values in the set {0, 1/(p-1), 2/(p-1), …, 1}. Then the experimental space $\Omega \subset ℜ^k$ forms k-dimensional p-level grid. Let Δ depend on p (an even number for convenience) and describe the side length of the grid element:

$$\Delta := 1/(p-1) \tag{3}$$

The elementary effect of the ith factor at a given point **x** is defined as:

$$d_i(\mathbf{x}) := \frac{y(x_1,\dots,x_{i-1},x_i+\Delta,x_{i+1},\dots,x_k)-y(\mathbf{x})}{\Delta} \tag{4}$$

Vector **x** is any point from Ω region such that the perturbed point **x** + Δ is still in Ω. A finite distribution F_i of elementary effect calculated for the ith factor is found by sampling **x** in Ω. The number of F_i values of each factor is $p^{k-1}[p-\Delta(p-1)]$ for k-dimensional p-level grid.

The distribution F_i can be described by mean and standard deviation, the values which characterize the influence of the ith factor on the model output.

Algorithm of trajectory generated in the parameter space.

Step 1. Select randomly start vector $\mathbf{x}^*$ such that each component $x_i \in \{0, 1/(p-1), \dots, 1-\Delta\}$, $i = 1 \dots k$.

Step 2. Increase one or more of k components of $\mathbf{x}^*$ by Δ such that the new vector $\mathbf{x}^{(1)}$ is still in Ω.

Step 3. Calculate elementary effect $d_i(\mathbf{x}^{(1)})$ following equation (4):

$$d_i\left(\mathbf{x}^{(1)}\right) = \frac{y(x_1^{(1)},\dots,x_{i-1}^{(1)},x_i^{(1)}\pm\Delta,x_{i+1}^{(1)},\dots,x_k^{(1)})-y(\mathbf{x}^{(1)})}{\Delta} \tag{5}$$

Step 4. Let $\mathbf{x}^{(2)}$ be the new vector $x_1^{(1)},\dots,x_{i-1}^{(1)},x_i^{(1)}\pm\Delta,x_{i+1}^{(1)},\dots,x_k^{(1)}$ defined in the step 3. Select the next vector $\mathbf{x}^{(3)}$ that differs from $\mathbf{x}^{(2)}$ for only one component j: $x_j^{(3)} = x_j^{(2)} \pm \Delta$ and $i \neq j$. Calculate elementary effect of the jth factor:

$$d_i\left(\mathbf{x}^{(2)}\right) = \begin{cases} \dfrac{y\left(\mathbf{x}^{(3)}\right)-y\left(\mathbf{x}^{(2)}\right)}{\Delta} & \Delta > 0 \\ \dfrac{y\left(\mathbf{x}^{(2)}\right)-y\left(\mathbf{x}^{(3)}\right)}{\Delta} & \text{otherwise} \end{cases} \tag{6}$$

Step 5. Repeat step 4 until $k + 1$ input vectors $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(k+1)}$ are generated. In the produced set of vectors called trajectory in the parameter space, every two consecutive vectors differ in only one component. One set of $k + 1$ vectors $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(k+1)}$ forms orientation matrix $\mathbf{B}^*$ of $(k + 1) \times k$ dimensions.

Algorithm of randomly selected orientation matrix $\mathbf{B}^*$.

Step 1. Select matrix **B** of $(k + 1) \times k$ dimensions with elements b_{ij} equal 0 or 1 ($i = 1 \dots k+1, j = 1 \dots k$) and every two columns of the matrix differ in only one element. In particular, **B** may be defined as a strictly lower triangular matrix with values of 1.

Step. 2. Build diagonal k dimensional matrix $\mathbf{D}^*$ such that:

$$d'_{ij} = \begin{cases} \pm 1 & i = j \quad \text{with equal probabilty} \\ 0 & i \neq j \end{cases} \tag{7}$$

Step 3. Build random permutation matrix $\mathbf{P}^*$ of $k \times k$ dimensions such that every column contains one element equal 1 and others equal 0 and there are no two columns which have values of 1 at the same position. In particular $\mathbf{P}^* = \mathbf{I}$.

Step 4. Build the matrix $\mathbf{B}^*$ following the formula:

$$\mathbf{B}^* = \left(\mathbf{J}_{k+1,1}\mathbf{x}^* + (\Delta/2)\left[\left(2\mathbf{B} - \mathbf{J}_{k+1,k}\right)\mathbf{D}^* + \mathbf{J}_{k+1,k}\right]\right)\mathbf{P}^* \tag{8}$$

where $\mathbf{J}_{k+1,1}$ and $\mathbf{J}_{k+1,k}$ are matrices with values 1 of dimensions appropriate $(k + 1) \times 1$ and $(k + 1) \times k$. Orientation matrix $\mathbf{B}^*$ provides a single elementary effect per factor.

Algorithm of estimation of mean and variance of the distribution F_i, $i = 1 \dots k$.

Step 1. Run r times algorithm of randomly selected orientation matrix $\mathbf{B}^*$, each for different starting point $\mathbf{x}^*$. It provides r independent orientation matrices with different trajectories for k factors, what is equivalent to r values for distribution F_i for each factor $i = 1 \dots k$.

Step 2. Since the trajectories are independent and they give independent estimators, estimate the mean μ and standard deviation σ for each of the factor through the classic estimators for independent random samples.

4. CALCULATIONS

The process that is considered as a case study for application of the mentioned method is a simple shearing test presented in figure 2. Selected material is OFHC copper deformed at the room temperature. The Morris design presented in chapter 3 is applied to the CAFE model described in chapter 2. Three factors are selected to the analysis: two parameters of the cellular automata module – as the crucial parameters in the micro shear bands development (equation (1)) and friction coefficient $\underline{\mu}$ that characterizes specimen-tool contact properties implemented in the Forge2 software. Thus, the vector $\mathbf{x}$ containing the parameters is in the following form:

$$\mathbf{x} = \left(x, \sigma_{dev}, \underline{\mu}\right) \tag{9}$$

where: x and σ_{dev} – expected value and standard deviation in equation (1), $\underline{\mu}$ – friction coefficient. The space of acceptable values for components of vector $\mathbf{x}$ is defined as: $x \in \langle 200, 500 \rangle$ MPa, $\sigma_{dev} \in \langle 10, 300 \rangle$ MPa, $\underline{\mu} \in \langle 0, 0.80 \rangle$.

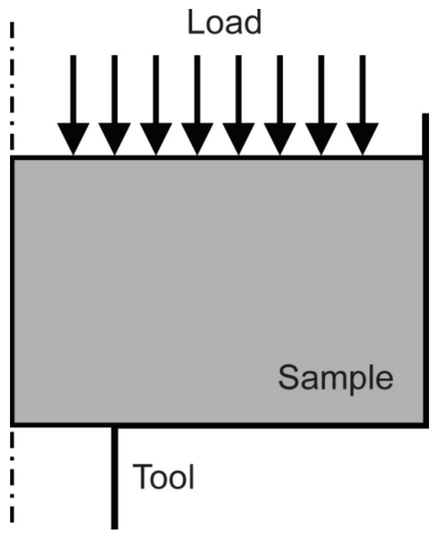


Fig. 2. *Simple shearing test with rectangular sample.*

The distribution of the strain values along the profile line at the fixed time of the process is analyzed to estimate the sensitivity (see figure 3). The strain profile is divided into two regions in such a way that the characteristic picks are observed. The output of the model is defined as the sum of the two relative strain picks:

$$y(\mathbf{x}) = \beta_1 y_1(\mathbf{x}) + \beta_2 y_2(\mathbf{x}) \tag{10}$$

where β_1, β_2 – coefficients such that $\beta_1 + \beta_2 = 1$ and for calculations in the present work the coefficients were assumed $\beta_1 = \beta_2 = 0.5$ – similar significance of the both strain picks, $y_i(\mathbf{x})$ $(i = 1,2)$ – relative strain pick, given by the formula:

$$y_i(\mathbf{x}) = \frac{\varepsilon_i^{\max}(\mathbf{x}) - \varepsilon_i^{\min}(\mathbf{x})}{\varepsilon_i^{\max}(\mathbf{x})} \qquad i = 1,2 \tag{11}$$

where $\varepsilon_i^{\max}(\mathbf{x}), \varepsilon_i^{\min}(\mathbf{x}), (i = 1,2)$, the maximum and the minimum of the strain along the fixed line for the first and the second strain region.

For the convenience of the calculation based on the Morris design, each factor of $\mathbf{x}$ vector is rescaled to the interval $\langle 0, 1 \rangle$. The parameters of the algorithm are setup as follows: the number of analyzed parameters k – 3, the number that characterizes the division of the unit interval p – 4, e.t. $\Delta = \left\{0, \frac{1}{3}, \frac{2}{3}, 1\right\}$, the number of independent trajectories r – 5. The results of sensitivity calculations are presented in figures 4 and 5.

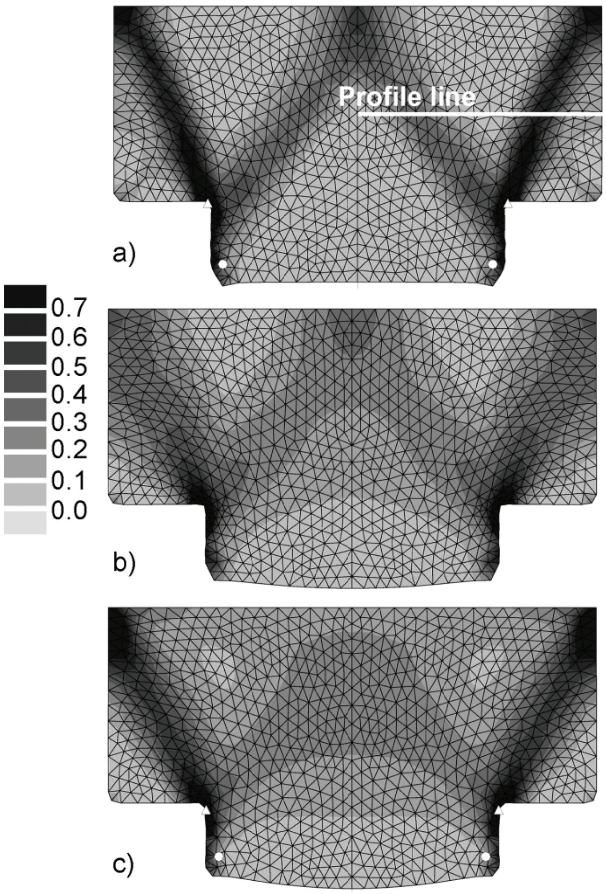
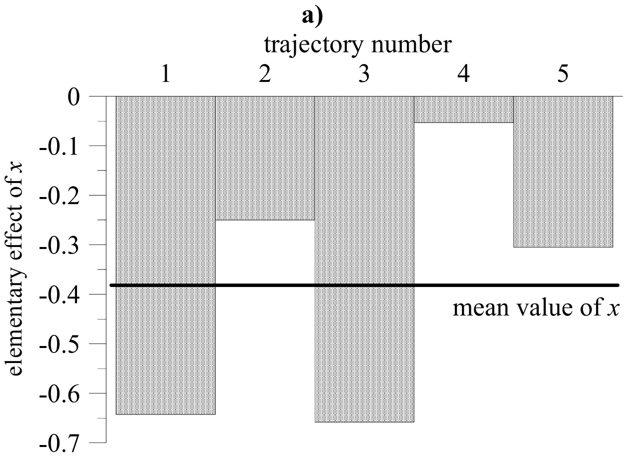


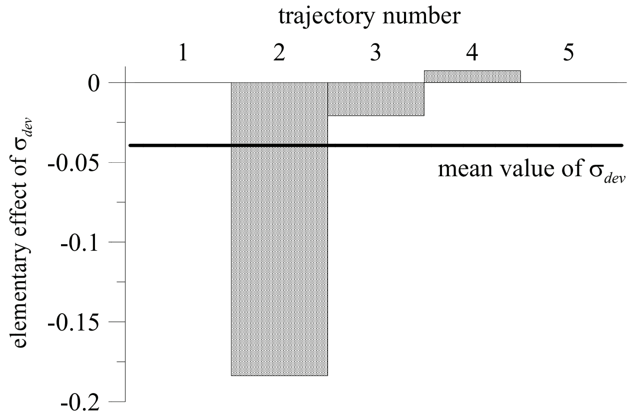
Fig. 3. Examples of strain distribution field obtained from the CAFE model with different input parameters: a) x = 200MPa, σ_{dev} = 300MPa, μ = 0, b) x = 400MPa, σ_{dev} = 107MPa, μ = 0, c) x = 400MPa, σ_{dev} = 107MPa, μ = 0.53.

a)



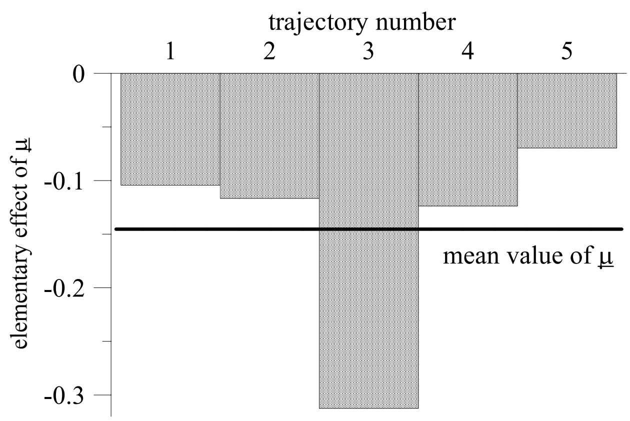
trajectory	x, MPa		σ_{dev}, MPa	μ, –
1	200	400	300	0.0
2	500	300	10	0.53
3	400	200	203	0.0
4	500	300	203	0.8
5	200	400	107	0.8

b)



trajectory	x, MPa	σ_{dev}, MPa		μ, –
1	400	300	107	0.0
2	300	10	203	0.53
3	200	203	10	0.0
4	300	203	10	0.8
5	400	107	300	0.8

c)



trajectory	x, MPa	σ_{dev}, MPa	μ, –	
1	400	107	0.0	0.53
2	300	203	0.53	0.0
3	200	10	0.0	0.53
4	300	10	0.8	0.27
5	400	300	0.8	0.27

*Fig. 4. Distribution F_i of the elementary effect d_i(**x**) for factors: a) expected value x, b) standard deviation σ_{dev}, c) friction coefficient μ. The values in tables indicate parameters x, σ_{dev}, μ, elementary effects were estimated on.*

5. DISCUSSION

The elementary effects of the expected value x (figure 4a) vary from -0.65 to -0.05. The highest values are obtained for conditions of the process while fraction of shear bands in the deformation is significantly independent of contact properties (friction coefficient) – see trajectories 1 and 3. The elementary effects of standard deviation σ_{dev} (figure

4b) vary from -0.18 to 0.07. If the values of the standard deviation are high the output of the model is not sensitive to this parameter (trajectories 1 and 5) or the response is weak (trajectories 3 and 4). The elementary effects of friction coefficient μ (figure 4c) vary from -0.31 to -0.06. The distribution is uniform except the trajectory 3 while the fraction of shear bands in the deformed specimen is very high.

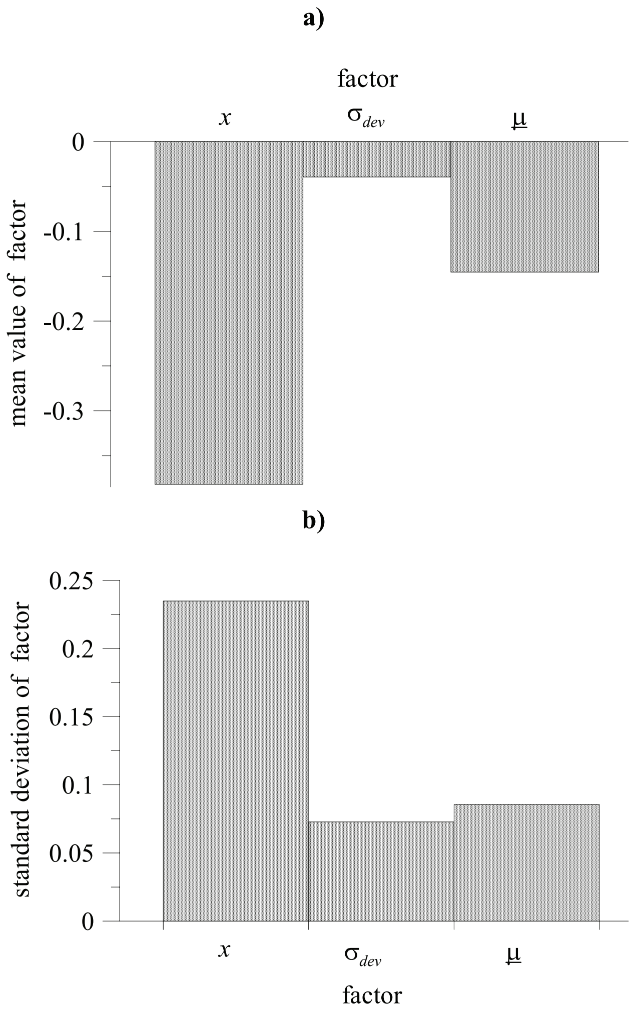


Fig. 5. a) Mean values and b) standard deviations for factors x, σ_{dev}, μ estimated based on Morris design.

The analysis of the mean values (figure 5a) proved that the model response is the most sensitive to the expected value x, the friction coefficient controls the process in minor extent and the influence of the standard deviation is weak. Standard deviations (figure 5b) of considered parameters show that expected value x with the highest value interact with other parameters (standard deviation σ_{dev} and friction coefficient μ) or its effect is nonlinear.

6. CONCLUSIONS

Application of the shearing test, where material flow is highly constrained provides valuable data for the sensitivity analysis, however another version of this test where one side of the sample is considered as free edge will be investigated too. The Morris algorithm of the screening design applied to the sensitivity analysis of the CAFE model highlighted the model parameters with the most important overall influence on the output. The main advantage of the Morris algorithm is the relatively low costs of calculations. This feature of the method is desirable due to excessive time of the CAFE simulation of complex deformation processes. The disadvantage is that interaction between the factors can not be estimated. The next step of the research will be application of other methods of sensitivity analysis to the CAFE model and comparison of the results. Second goal is to explore other parameters and the areas of factors space where model response is the most significant. As presented the influence of the standard deviation is very small that is why during further research investigation of additional parameters that are present in the transition rules have to be considered. As expected value of x is the most significant and this value have to be identified very precisely to properly describe real material behaviour. Obtained results will be helpful in the inverse analysis to identify the model parameters using efficient optimization algorithms and to predict the material behaviour during the process with higher accuracy.

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ANALIZA WRAŻLIWOŚCI WIELOSKALOWEGO MODELU ZJAWISKA LOKALIZACJI ODKSZTAŁCENIA BAZUJĄCEGO NA METODZIE CAFE

Streszczenie

Celem niniejszej pracy jest zastosowanie analizy wrażliwości do określenia wpływu parametrów modelu wieloskalowego CAFE na wyniki symulacji procesu odkształcania związane z lokalizacją odkształcenia. W tym celu przeprowadzono szereg symulacji numerycznych, które posłużyły jako dane wejściowe do analizy wrażliwości metodą Morrisa. W pracy umieszczono opis zastosowanej metody Morisa, omówiono także jej zalety jak i wady. Wyniki przeprowadzonej analizy stanowią podstawę do dyskusji nad kierunkami dalszych badań obejmujących wykorzystanie metody analizy odwrotnej do identyfikacji parametrów modelu CAFE.

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