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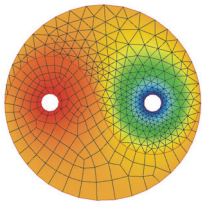

THE USE OF MORRIS METHOD IN SENSITIVITY ANALYSIS OF THE NUMERIC MODEL OF SOLIDIFICATION

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Abstract

In this work use of the Morris method in sensitivity analysis of a numerical model of solidification is discussed. Sensitivity analysis permits to study influence of model parameters on the results, which makes it possible to determine which parameters have considerable influence and which are insignificant. The Morris method is suitable for analysis of computationally expensive models with great number of parameters, as it involves small number of model computations. Sensitivity of a numerical model of solidification developed by the authors is studied as a numerical example.

Key words: sensitivity analysis, Morris method, computer experiment, finite element method, solidification model

1. INTRODUCTION

Numerical models which are created nowadays can be characterised by a high degree of complication. This complication concerns mainly, among other things, large number of parameters in a model. It turns out, however, that individual parameters often have different influence on the results of computations. Variation of some parameters causes substantial change in the results, whereas changing the others has marginal effect. Since the model parameters are often the material properties which have to be actually measured, knowing which parameters are less relevant allows to save tedious experimental work. On the other hand, the parameters with the largest influence on the results can be determined or measured more exactly to be included in the model with greater accuracy.

Sensitivity analysis deals with the problem of ranking of model parameters on the basis of their influence on the received results. Both local and global approaches to the analysis are possible. In the local approach the goal is to assess influence of change of an individual parameter while keeping the other parameters fixed. In the global approach these other parameters are also subject to change. Many methods exist for the global analysis, varying among other things in computational cost. The Morris method belongs to this group and is the subject of this paper.

One of the advantages of the Morris method is its low computational cost, which means possibility to obtain sensitivity results with relatively small computational effort. This feature enables usage of the method for models with many parameters and with long computation times. An example of such a problem is solidification. This is the long time of process simulation and great number of solidification model parameters that were the reasons for selecting the Morris method for sensitivity analysis.

In the presented work a solidification solver developed in the Institute of Computer and Information Sciences at Czestochowa University of Technology is analyzed. The executed sensitivity analysis permits to rank model parameters with respect to their

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influence on the received results. This knowledge allows to distinguish the particularly important parameters from those with little influence.

2. THE MORRIS METHOD

Sensitivity analysis method applied in this work is based on the Morris method, which is described in detail in Morris (1991) or in Saltelli et al. (2004).

Consider a model $y = y(\mathbf{x})$, where $\mathbf{x}$ is the vector of model parameters. It is possible to create a matrix $\mathbf{B}^*$ given by

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

where k is the number of parameters, $\mathbf{J}_{m,k}$ and $\mathbf{J}_{m,1}$ are matrices of ones, $m=k+1$, $\mathbf{D}^*$ is a diagonal matrix of the size m with the values +1 and -1 distributed in the diagonal with equal probability, $\mathbf{B}$ is a m times k matrix with ones below the diagonal and zero elsewhere, and $\mathbf{P}^*$ is a square random permutation matrix of the size k. Each column of this matrix contains only one element with the value +1 while the remaining elements are equal to zero. Row index of +1 in a column is unique for this column within the matrix.

The $\mathbf{x}^*$ vector of the size k contains values randomly selected from the set $\{0, 1/(p-1), 2/(p-1), \ldots, 1-\Delta\}$, assuming equal probability of selection, in which

$$\Delta = \frac{1}{p-1} \quad (2)$$

and p is the number of points used to subdivide the interval of variation of a model parameter (all parameters are normalized to vary between 0 and 1).

The $\mathbf{B}^*$ matrix evaluated using the formula (1) has the following features: each of its rows is a set of model parameters, all the elements are in the range from 0 to 1, each row pair differs by Δ or $-\Delta$ in exactly one element. Matrix elements must be scaled to conform to the original interval of parameters variation, similarly the Δ.

Once the $\mathbf{B}^*$ matrix is built, it is possible to calculate the following quotients

$$d_i(x) = \frac{y(x_1, x_2, \ldots, x_{i-1}, x_i + \Delta, x_{i+1}, \ldots, x_k) - y(\mathbf{x})}{\Delta} \quad (3)$$

$$d_i(x) = \frac{y(\mathbf{x}) - y(x_1, x_2, \ldots, x_{i-1}, x_i - \Delta, x_{i+1}, \ldots, x_k)}{\Delta} \quad (4)$$

Arguments of the model function y are taken from the two successive rows of the $\mathbf{B}^*$ matrix, differing in the ith element by Δ. If Δ was added to a parameter then the formula (3) is used, whereas the formula (4) is for the case when the parameter was decreased by that value.

The value of d_i is an indicator of how significant the parameter is. Obviously, greater d_i means higher sensitivity of the results to the changes in the ith parameter.

Full sensitivity analysis with the Morris method requires several repetitions of the steps described in previous paragraphs. Then, assuming that creation of matrix $\mathbf{B}^*$ was done r times, influence of the ith parameter is calculated as an average taken from all repetitions

$$\mu_i = \frac{1}{r}\sum_{j=1}^{r} d_{ij} \quad (5)$$

Additionally, it is possible to calculate standard deviation for this parameter as

$$\sigma_i = \sqrt{\frac{1}{r}\sum_{j=1}^{r}\left(d_{ij} - \mu_i\right)^2} \quad (6)$$

Nonzero values of σ_i indicate nonlinear influence of the parameter. It is also a sign of interaction among individual parameters.

In the presented work the formulas (3) and (4) for the quotients have been modified in order to make the results for different parameters comparable, as their values may differ in orders of magnitude. The quotients were evaluated from

$$d_i(x) = \frac{\dfrac{y(x_1, x_2, \ldots, x_{i-1}, x_i \pm \Delta, x_{i+1}, \ldots, x_k) - y(\mathbf{x})}{y(\mathbf{x})}}{\dfrac{(x_i \pm \Delta) - x_i}{x_i}} \quad (7)$$

This modification ensures that d_i does not become large for parameter with small value, because for that parameter Δ also is small. If formulas (3) or (4) have been used, d_i would become large, despite small value of difference in numerator.

3. NUMERICAL MODEL UNDER STUDY

As it was mentioned in the introduction, sensitivity of a numerical model of solidification was analyzed as an example of using the Morris method. The model was implemented in a solver being part of the *NuscaS* software package and is described in Sczygiol (2000).

It is based on the heat transfer equation with a heat source involving release of latent heat of solidification

$$\nabla \cdot (\lambda \nabla T) + \dot{q} = c\rho \frac{\partial T}{\partial t} \tag{8}$$

where

$$\dot{q} = \rho_s L \frac{\partial f_s}{\partial t}, \tag{9}$$

λ is thermal conductivity, c is specific heat, ρ is density, L is latent heat, t is time, T is temperature and f_s is solid mass fraction (subscript s denotes the solid phase, and l denotes the liquid phase). Introducing the enthalpy H makes it possible to rewrite the heat equation in source-free form

$$\nabla \cdot (\lambda \nabla T) = \frac{\partial H}{\partial t} \tag{10}$$

where for a metal alloy solidifying in the temperature range (T_L-T_S) the enthalpy is defined as

$$H = \begin{cases} \int_{T_{ref}}^{T} c\rho_s dT, & T < T_S \\ \int_{T_{ref}}^{T_S} c\rho_s dT + \int_{T_S}^{T} \left(c\rho_f - \rho_s L \frac{\partial f_s}{\partial T} \right) dT, & T_S \le T \le T_L \\ \int_{T_{ref}}^{T_S} c\rho_s dT + \rho_s L + \int_{T_S}^{T_L} c\rho_f dT + \int_{T_{Lf}}^{T} c\rho_l dT, & T > T_L \end{cases} \tag{11}$$

where the subscript f denotes the two-phase region.

The equation (10) was solved using the finite element method. As the result of spatial discretization the following system of ordinary differential equation is obtained

$$\mathbf{M}\dot{\mathbf{H}} + \mathbf{K}(T)\mathbf{T} = \mathbf{b}(T) \tag{12}$$

where **M** denotes the mass matrix, **K** denotes the conductivity matrix, **T** is the nodal temperature vector, **H** denotes the enthalpy vector and **b** is the vector including contributions from boundary conditions. Elements of these matrices and of the right-hand side vector are calculated from the following formulas (for one finite element)

$$\begin{aligned} \mathbf{M}^e &= \int_{\Omega^e} \mathbf{N}^T \mathbf{N} d\Omega \\ \mathbf{K}^e &= \int_{\Omega^e} \lambda(T) \nabla^T \mathbf{N} \cdot \nabla \mathbf{N} d\Omega \\ \mathbf{b}^e &= \int_{\Gamma} \mathbf{N}_\Gamma^T \mathbf{N}_\Gamma d\Gamma \, \mathbf{q}^T(T) \end{aligned} \tag{13}$$

where **N** is a vector of shape functions of this finite element in domain Ω, $\boldsymbol{N}_\Gamma$ denotes a vector of shape functions on the boundary Γ and **q** denotes the nodal heat flux vector.

Equation (12), which contains the time derivative, was integrated in time with use of the two-step Dupont II method and the following system of algebraic equations (14) was obtained:

$$\left(\mathbf{M} + \frac{3}{4}\Delta t \mathbf{K}^0 \left[\frac{d\mathbf{T}}{d\mathbf{H}} \right]^{n+1} \right) \mathbf{H}^{n+2} = \left(\mathbf{M} + \frac{3}{4}\Delta t \mathbf{K}^0 \left[\frac{d\mathbf{T}}{d\mathbf{H}} \right]^{n+1} \right) \mathbf{H}^{n+1} - \\ - \frac{3}{4}\Delta t \mathbf{K}^0 \mathbf{T}^{n+1} - \frac{1}{4}\Delta t \mathbf{K}^0 \mathbf{T}^n + \frac{3}{4}\Delta t \mathbf{b}^{n+2} + \frac{1}{4}\Delta t \mathbf{b}^n \tag{14}$$

where the superscript denotes time step number. The zero superscript means that a quantity is calculated for material properties at the extrapolated temperature:

$$T = \frac{3}{2}T^{n+1} - \frac{1}{2}T^n \tag{15}$$

Elements of the diagonal matrix are calculated from:

$$\frac{dT}{dH} = \begin{cases} \frac{1}{c\rho_s}, & T < T_S \\ \frac{1}{c\rho_f - \rho_s L \frac{df_s}{dT}}, & T_S \le T \le T_L \\ \frac{1}{c\rho_l}, & T > T_L \end{cases} \tag{16}$$

The quantity f_s, which appears in the formula (16), depends on the assumed solidification model (equilibrium, nonequilibrium or intermediate) and is calculated utilizing dependencies from the phase diagram. Since the intermediate model of solid phase growth was assumed, the solid phase fraction is calculated from the formula

$$f_s(T) = \frac{1}{1 - nk\alpha} \left(1 - \left(\frac{T_M - T}{T_M - T_L} \right)^{\frac{1 - nk\alpha}{k-1}} \right) \tag{17}$$

where k denotes the equilibrium partition ratio, T_M denotes the fusion temperature for pure base component, T_L denotes the liquidus temperature, α denotes the Brody-Flemmings coefficient, and n is a coefficient, which depends on grain shape. For flat grains this coefficient equals n=2.

The heat equation (10) must be accompanied by appropriate boundary conditions. It was assumed that heat can be exchanged with the environment through external boundary Γ where the boundary condition of the third type is defined as

$$\Gamma: \quad q = \alpha\left(T - T_{\infty}\right) \tag{18}$$

where α denotes the coefficient of heat exchange between the boundary with the temperature T and the environment with ambient temperature T_{∞}.

The other boundary condition used in this work is the boundary condition of the fourth type, which represents heat flux through the internal boundary Γ which separates the cast from the mold. In case the contact is through a separating layer of the thickness δ, the condition is given by

$$\Gamma: \begin{cases} -\left(\mathbf{n}\cdot\lambda\nabla T\right)^{(1)} = -\left(\mathbf{n}\cdot\lambda\nabla T\right)^{(2)} = \dfrac{\lambda_p}{\delta}\left(T^{(1)} - T^{(2)}\right) \\ T^{(1)} \neq T^{(2)} \end{cases} \tag{19}$$

where λ_p denotes heat transfer coefficient of the layer.

5. RESULTS OF NUMERICAL EXPERIMENTS

Numerical experiments were performed on the model described in the previous chapter. Values of the parameters that have been used are summarized in tables 1 and 2.

Table 1 contains only those parameters that were subject to change within an interval. The interval was defined by the minimal and the maximal value and was divided by four points (p=4). The **B*** matrix was evaluated ten times (r=10). As the number of necessary simulation runs is equal to $r(k + 1)$, the solidification solver was executed 80 times.

Table 2 contains the values of the parameters which were fixed during sensitivity analysis. Their influence was not investigated because their relationships are very hard to express using simple mathematical rules. Random changes, even in small limited intervals, can cause results noncompliant with the nature of the simulated phenomenon.

The solidification time was selected as the model output. It is defined as the time interval from the beginning of the simulation until the moment when the last portion of the casting domain is passed by the solidus isotherm. Computed solidification times varied from 834s to 1999.2s.

In figures 1 and 2 results obtained from sensitivity analysis of the solidification model are presented. Numbers 1-7 in these figures correspond to the numbers from the first column of table 1.

The graph presented in figure 2 shows sensitivity in the (average, standard deviation) coordinate sys tem.

Table 1. *Variable model parameters.*

Index	Minimal Value	Maximal Value	Physical Unit	Parameter Name
1	2080	3120	kg/m^3	density of casting
2	800	1200	J/(kg K)	specific heat of casting
3	80	120	W/(m K)	thermal conductivity of casting
4	312000	468000	J/kg	latent heat of fusion
5	2.4*10^{-9}	3.6*10^{-9}	m^2	Brody-Flemmings coefficient
6	800	1200	W/(m^2 K)	heat transfer coefficient between the mold and the ambient air
7	800	1200	W/(m^2 K)	heat transfer coefficient between the casting and the mold

Table 2. *Physical properties which influence on the results was not investigated.*

Value	Physical Unit	Parameter Name
7200	kg/m^3	density of mold
738	J/(kg K)	specific heat of mold
30	W/(m K)	thermal conductivity of mold
853	K	solidus temperature
923	K	liquidus temperature
933	K	fusion temperature for pure base metal
821	K	eutectic temperature
0.125	---	equilibrium partition ratio
300	K	temperature of the ambient air

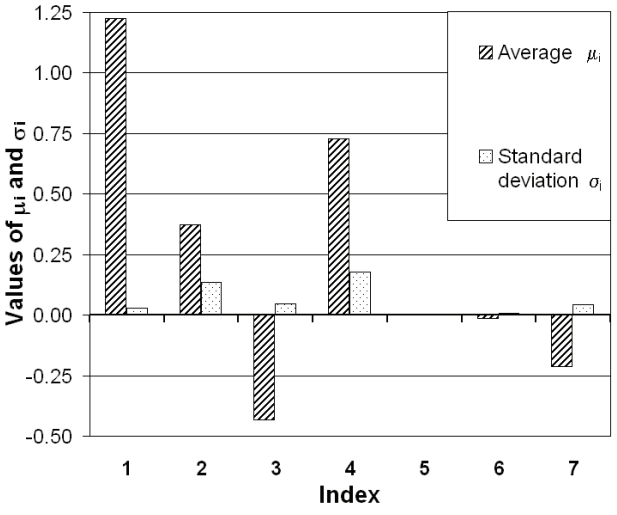

Fig. 1. *Values of sensitivity for the given parameters. Symbols 1-7 correspond to the labels from the first column of table 1.*

Each point of this graph represents values of sensitivity for one parameter. These points are labeled by numbers, which correspond to the first column of table 1.

Negative sign in average values of the indicator d_i for some parameters (3, 6, 7) means that increase of such a parameter results in decrease in the model output.

As it can be seen in the presented figures, the following parameters have the largest influence on solidification time: density of the casting and latent heat of fusion (parameters 1 and 4). It is also impossible to ignore the influence of heat conductivity, and specific heat of the casting, as well as heat transfer coefficient between the casting and the mold (parameters 2, 3, and 7). Parameters which have very little influence on the model output are the Brody-Flemmings coefficient and heat transfer coefficient between the mold and ambient air (parameters 5 and 6).

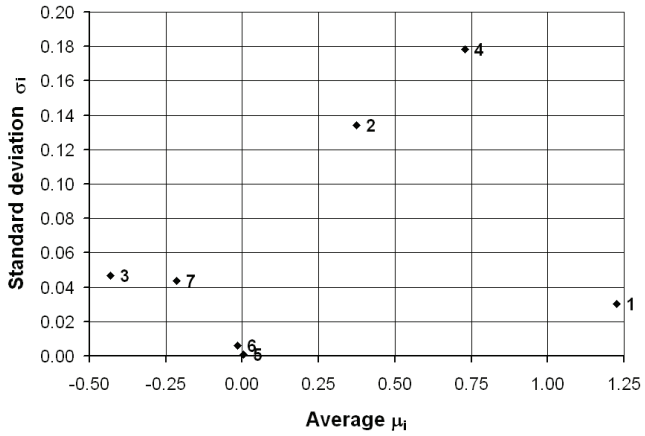

Fig. 2. *Values of sensitivity of the investigated parameters. The meaning of symbols 1-7 is the same as in figure 1.*

6. CONCLUSIONS

Application of the Morris method to sensitivity analysis of the numerical model of solidification was presented in this work. Advantages of this method are capability of obtaining results with relatively small computational effort and also lack of necessity to modify the examined model. The results allow to differentiate parameters by their effect on the model output. Large influence of density and latent heat of fusion permits to assume that there is a connection between the phenomenon occurring during solidification of casting and the solidification time in the given model.

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ZASTOSOWANIE METODY MORRISA DO ANALIZY WRAŻLIWOŚCI NUMERYCZNEGO MODELU KRZEPNIĘCIA

Streszczenie

W przedstawionej pracy zamieszczone jest omówienie analizy wrażliwości numerycznego modelu krzepnięcia za pomocą metody Morrisa. Analiza wrażliwości pozwala na badanie wpływu poszczególnych parametrów na uzyskiwane wyniki. Pozwala to ustalić parametry, które mają znaczny wpływ na wyniki, jak również te, których wpływ jest niewielki. Metoda Morrisa jest szczególnie przydatna do badania modeli, które wymagają dużego nakładu obliczeń lub są opisane dużą liczbą parametrów, z powodu niewielkiej wymaganej przez nią wykonanych symulacji komputerowych. Analiza wrażliwości numerycznego modelu krzepnięcia opracowanego przez autorów pracy jest przedstawiona jako przykład zastosowania metody Morrisa.

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