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THE APPLICATION OF THE MORRIS METHOD FOR DETERMINATION OF RANGES OF PARAMETERS VARIATION, HAVING ASSUMED INFLUENCE ON CALCULATION RESULT

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Abstract

A method of sensitivity analysis for determining acceptable ranges of uncertainty of tested model's parameters was presented in this paper. Our approach is based on Morris method with modified sensitivity indicator. Solver from NuscaS system, which enables making simulation of casts solidification made from two-component alloys was used as a model. This model is built on the basis of the finite elements method, which is used to solve thermal conduction problem. Enthalpy formulation was used by the considered model. Acceptable ranges of parameters' uncertainty are determined in the way that parameters' values increases caused previously assumed changes of resulting quantity.

Key words: sensitivity analysis, simulation of solidification, finite elements method, material properties

1. INTRODUCTION

Simulation of solidification, with modern models, is connected with determination of high number of physical parameters. This situation appears because presently created models of physical phenomena proceeding in solidifying casts are more complicated. Nevertheless, it seems that not all used parameters have equal impact on results. Sensitivity analysis is use to determine which parameter has the greatest impact on the model, and which one has the least impact. This paper shows how to use one of sensitivity analysis methods. The information concerning with how high uncertainty may experimental model's parameters be determined, so that all parameters caused equal result's deviation, was taken into account.

2. INSPECTED MODEL

Solver of NuscaS system (Sczygiol, 2000), which enables making simulation of phenomena occurring in solidifying casts was choosen as a considered model. This solver is based on the equation of thermal conduction with heat source. This equation is solved with the use of enthalpy solidification formulation (Sczygiol & Szwarc, 2001). It is transformed into system of equations that contains only time differential. This transformation is realized by using finite elements method. Time integration goes on with the use of Dupont II two-steps scheme of integration (Wood, 1990). Modified Euler's backward scheme was used for the calculation of the solution of first time step. NuscaS enables using of different models of solid phase growth. The user can choose between equilibrium, non-equilibrium and indirect model of solid phase growth. All simula-

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tions described in this paper were carried out with the use of indirect model of solid phase growth.

3. THE DESCRIPTION OF MORRIS METHOD

Determination of acceptable ranges of parameters uncertainty is based mainly on the Morris method. Description of this method is briefly presented in this chapter. Much more comprehensive description can be found in literature, for example in Morris article (1991) or Saltelli's et al. textbook (2004).

The essence of Morris method is to create matrix containing adequately prepared sets of model's parameters. It is assumed that we are taking into the model described by equation $y = y(\mathrm{x})$, where x is a vector of model's parameters. Creation of this matrix, marked further as B*, starts from establishing basic parameters, such as the number of inspected model's parameters, marked by k and the number of sub-ranges, that determines for how many parts is divided the range of variation for given parameter. The number of sub-ranges, increased by one, is marked as parameter p. All sub-domains are the same length, that is marked by Δ. B* matrix is created on a basis of the following formula:

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

The vector x*, that consists of k elements, is created as the result of random sampling. Each of its elements is randomly chosen from $\left\{0, 1, \frac{1}{p-1}, \frac{2}{p-2}, \ldots, 1-\Delta\right\}$ set with the equal probability of choosing.

$\mathrm{J}_{m,k}$ matrix is completely filled with values 1. Its sizes are: m rows and k columns, where $m=k+1$. Analogically, $\mathrm{J}_{m,1}$ vector is also completely filled with elements with the value of 1. It consists of m elements.

In matrix B, there are ones only below main diagonal. Other of elements are equal 0.

Elements of D* matrix lying on principal diagonal are sampled from set $\{-1, 1\}$, where both elements from the set has equal probability of occurring. The rest of elements is equal to 0. Matrix D* is a square matrix with size m

P* matrix, that is a square matrix with k size, is defined as the matrix of random permutations. Each column in this matrix contains accurately one element with the value of 1 and none of two columns have elements equal to 1 in the same place. Elements of this matrix, which are not equal to 1, have the value of 0.

B* matrix, created in described way, has following properties: each of its rows responds to the set of model's parameters, all its elements have values from the range from 0 to 1, only one element in two neighboring rows differs in Δ (both increase and decrease of this value may occur there). Because all elements of B* matrix are from the range from 0 to 1, so it is possible to make re-scaling, so that their values respond to the values of used parameters. This rule can be also applied to the value of Δ.

After creation of B* matrix and scaling values of its particular elements, the quotients can be determined from the following formula (Sczygiol & Dyja, 2007):

$$d_i(\mathrm{x}) = \frac{y(x_1, x_2, \ldots, x_{i-1}, x_i \pm \Delta, x_{i+1}, \ldots, x_k) - y(\mathrm{x})}{\pm\Delta} \frac{x_i}{y(\mathrm{x})} \quad (2)$$

The quantity d_i is used to determine the indicators, that give information how big is the impact of given parameters on results of simulation.

Complete sensitivity analysis with Morris' method (1991) requires more than one creation of B* matrix. It assures that for each parameter exists r values of d_i (r – the number of generated B* matrices). Absolute value of their mean, marked as μ_i, gives information how big is the impact of given parameter's. The greater mean value is, the greater is the impact of given parameter on results of simulation.

Additionally, σ value of standard deviation is also computed, which non-zero value informs about non-linear impact of given parameter. It is also the symptom of proceeding the interaction between individual parameters.

Although there is an improvement of used method called new Morris method (Campolongo & Braddock, 1999), we decided to use standard Morris method. The new one has a few interesting features, but does not offer great improvement in accuracy of results of μ values. Moreover implementation of new Morris method is difficult and this method requires more model evaluations than standard method.

4. DESCRIPTION OF THE MODIFICATION

Information about the model, obtained in the process of sensitivity analysis can be used to determine ranges of uncertainty of model's parameters so as the changes of all parameters in these ranges caused equal changes of results obtained from the simulation. The following formula can be used for calculation of new values of parameters' increases:

$$\Delta_i' = \frac{a}{\mu_i'}\Delta \qquad (3)$$

where μ_i' value is the mean of indices d_i' that are calculated in the following way:

$$d_i' = \left| y(x_1, x_2, \ldots, x_{i-1}, x_i \pm \Delta, x_{i+1}, \ldots, x_m) - y(x_1, x_2, \ldots, x_{i-1}, x_i, x_{i+1}, \ldots, x_m) \right| \qquad (4)$$

The parameter a is determined in advance and it represents given range of the result's uncertainty, i.e. how much the maximal resulting value may change.

Minimal and maximal values of parameters have to be changed in the same manner as the values of parameters' increase. One may obtain appropriate boundaries of the ranges through multiplication basic values with $\frac{a}{\mu'_i}$.

There should be emphasized, that these calculations do not require any additional simulations or modification of the way of samples' preparing and that is why they can be made after sensitivity analysis.

5. RESULTS OF EXPERIMENTS

Sensitivity analysis of the solver of NuscaS system was made, in order to practical illustration of considerations presented in previous paragraph. The impact of the parameters on the time of casting's solidification, was tested in the analysis. The parameters chosen for analysis are collected in table 1. Time of solidification was counted from the beginning of simulation up to the moment of solidification of the last part of material. Time of solidification was counted with accuracy 0.2 s. Values of parameters, which were not subject of sensitivity analysis, but which were necessary for execution of the simulation, are presented in table 2. Initial temperature of the casting was set to 1000K, while initial temperature of the mould was 300K.

Shape of the area, for which the calculations were performed, is shown in figure 1. The sector of the casting mould was presented, together with its dimensions. Domain of the problem was divided into 2304 finite elements, 616 of them are dedicated to the casting, while 1668 elements are dedicated to the mould. Triangular finite elements of first order were used. The shape of the problem's domain enabled usage of structural mesh of finite elements.

It was assumed, that there exists heat exchange between mould and environment through the boundary condition of third order (called also Newton's boundary condition). The contact between mould and casting is modeled with usage of the boundary condition of fourth order (continuity condition) with the consideration of non-ideal contact, i.e. the contact taking place through the separating layer. The boundary condition of second order with zero heat flux models axes of symmetry that occurs in the problem.

The results of original sensitivity analysis (of μ_i column and σ_i one) are shown in table 3. New variation ranges of considered parameters were calculated on the basis of analysis. Average time increases of the solidification, caused through the change of given parameter (column μ_i' calculated according to the formula (4)) are also placed in table 3. On the base of results collected in the table, it can be observed, that the highest sensitivity value is assumed for these parameters, which average increase of solidification time is the highest.

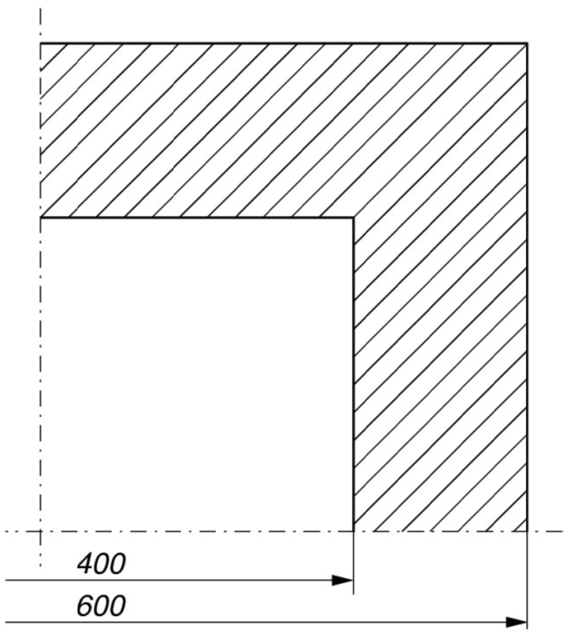

***Fig. 1.** The shape of domain, for which the calculations were carried out.*

Table 1. *Basic values of given parameters.*

Lp.	Name of the parameter	Minimal value	Central value	Maximal value	Δ_i	Unit
1	Casting material density	2080	2600	3120	346,67	kg/m^3
2	Casting material specific heat	800	1000	1200	133,33	J/(kg·K)
3	The coefficient of thermal conduction of the casting material	80	100	120	13,33	W/(m·K)
4	Latent heat of solidification	312000	390000	468000	52000	J/kg
5	Brody's-Flemmings coefficient	$2{,}4 \cdot 10^{-9}$	$3{,}0 \cdot 10^{-9}$	$3{,}6 \cdot 10^{-9}$	$0{,}40 \cdot 10^{-9}$	m^2
6	Coefficient of heat exchange between the mould and environment	800	1000	1200	133,33	W/(m^2·K)
7	Coefficient of heat exchange of the layer separating mould and casting	800	1000	1200	133,33	W/(m^2·K)

Table 2. *Physical parameters, not subjecting to changes, used in the model.*

Name of the parameter	Value	Unit
Solidus temperature	853	K
Liquidus temperature	923	K
Temperature of pure component solidification	933	K
Eutectic temperature	821	K
Coefficient of admixture separation	0,125	K
Ambient temperature	300	K
Mould material density	7200	kg/m^3
Mould material specific heat	738	J/(kg·K)
Thermal conductivity coefficient of mould material	30	W/(m·K)

Table 3. *The results of sensitivity analysis and average increase of solidification time.*

Lp.	Name of the parameter	μ_i	σ_i	μ_i'
1	Casting material density	1,2300	0,0262	215,06
2	Casting material specific heat	0,4060	0,0419	73,38
3	The coefficient of thermal conduction of the casting material	-0,4155	0,0521	74,82
4	Latent heat of solidification	0,8409	0,0451	125,66
5	Brody's-Flemmings coefficient	0,0024	0,0008	0,48
6	Coefficient of heat exchange between the mould and environment	-0,0120	0,0045	2,28
7	Coefficient of heat exchange of the layer separating mould and casting	-0,2473	0,0361	43,68

Table 4. *Values of parameters in the case of the assumption that time of casting solidification changes at one second on average.*

Lp.	Name of the parameter	Minimal value	Central value	Maximal value	Δ_i	Unit
1	Casting material density	2597,60	2600	2602,40	1,60	kg/m^3
2	Casting material specific heat	997,28	1000	1002,72	1,81	J/(kg·K)
3	The coefficient of thermal conduction of the casting material	99,73	100	100,27	0,18	W/(m·K)
4	Latent heat of solidification	389380	390000	390620	413,33	J/kg
5	Brody's-Flemmings coefficient	$1{,}75 \cdot 10^{-9}$	$3{,}0 \cdot 10^{-9}$	$4{,}25 \cdot 10^{-9}$	$8{,}33 \cdot 10^{-10}$	m^2
6	Coefficient of heat exchange between the mould and environment	912,28	1000	1087,72	58,48	W/(m^2·K)
7	Coefficient of heat exchange of the layer separating mould and casting	995,42	1000	1004,58	3,05	W/(m^2·K)

Table 5. *Values of parameters in the case of the assumption that time of casting solidification changes at two seconds on average.*

Lp.	Name of the parameter	Minimal value	Central value	Maximal value	Δ_i	Unit
1	Casting material density	2595,16	2600	2604,84	3,23	kg/m^3
2	Casting material specific heat	994,54	1000	1005,46	3,64	J/(kg·K)
3	The coefficient of thermal conduction of the casting material	99,47	100	100,53	0,35	W/(m·K)
4	Latent heat of solidification	388760	390000	391240	826,67	J/kg
5	Brody's-Flemmings coefficient	$0{,}5\cdot10^{-9}$	$3{,}0\cdot10^{-9}$	$5{,}5\cdot10^{-9}$	$1{,}67\cdot10^{-9}$	m^2
6	Coefficient of heat exchange between the mould and environment	824,48	1000	1175,52	117,01	W/(m^2·K)
7	Coefficient of heat exchange of the layer separating mould and casting	990,84	1000	1009,16	6,11	W/(m^2·K)

Table 6. *Values of parameters in the case of the assumption that time of casting solidification changes at ten seconds on average.*

Lp.	Name of the parameter	Minimal value	Central value	Maximal value	Δ_i	Unit
1	Casting material density	2576,00	2600	2624,00	16,00	kg/m^3
2	Casting material specific heat	972,80	1000	1027,20	18,13	J/(kg·K)
3	The coefficient of thermal conduction of the casting material	97,30	100	102,70	1,80	W/(m·K)
4	Latent heat of solidification	383800	390000	396200	4133,33	J/kg
5	Brody's-Flemmings coefficient	$0{,}5\cdot10^{-9}$	$3{,}0\cdot10^{-9}$	$5{,}5\cdot10^{-9}$	$1{,}67\cdot10^{-9}$	M^2
6	Coefficient of heat exchange between the mould and environment	122,80	1000	1877,20	584,80	W/(m^2·K)
7	Coefficient of heat exchange of the layer separating mould and casting	954,20	1000	1045,80	30,53	W/(m^2·K)

Table 7. *The results of sensitivity analysis and average increase of solidification time after modification of ranges of parameters' variation in the case of assumed increase at:: 1 – one second, 2 – two seconds, 3 – three seconds.*

Lp.	1			2			3		
	μ_i	σ_i	μ_i'	μ_i	σ_i	μ_i'	μ_i	σ_i	μ_i'
1	1,2308	0,1196	0,94	1,2735	0,0527	1,96	1,2458	0,0336	9,52
2	0,4358	0,0264	0,98	0,4388	0,0138	1,98	0,4447	0,0071	9,88
3	-0,4389	0,0269	0,98	-0,4284	0,0232	1,88	-0,4393	0,0069	9,88
4	0,8059	0,0690	1,06	0,8069	0,0377	2,12	0,7933	0,0128	10,44
5	0,0030	0,0009	1,12	0,0019	0,0008	2,12	0,0023	0,0017	2,20
6	-0,0114	0,0011	0,86	-0,0116	0,0008	1,78	-0,0136	0,0049	9,58
7	-0,2321	0,0262	0,88	-0,2412	0,0077	1,82	-0,2376	0,0091	9,00

Negative values of indicators occurs in the table for the following parameters: coefficient of thermal conductivity of the casting material, coefficient of heat exchange between the mould and environment, as well as coefficient of heat exchange of the layer separating mould and the casting. It is due to the situation where the increase of given parameters causes decrease of result value. Because in the formula (4) – in contradistinction to the formula (2) – absolute value is used all values in last column of table 3 are positive.

Table 4 contains new ranges of parameters variation, calculated on the basis of the results from table 3 with the use of formula (3). It was assumed, that time of solidification may increase of one second on the average. Successive tables contain values of parameters in the situation, when changes of all parameters cause average change of two seconds (table 5), or (with neglecting Brody's-Flemmings coefficient) of ten seconds (table 6). The variation range for Brody's-Flemmings coefficient, calculated in the last case, assumed negative value as a lower range. This was contradictory with values of that parameter that are acceptable by the model. Therefore one decided leave minimal and maximal values the same as in the case were changes of two seconds were assumed.

Table 7 presents results of sensitivity analysis in the case of use of modified ranges of parameters variation. The number of line in the table corresponds to the number of line from table 1. The results were grouped for three cases: average increase of solidification time by one, two and ten seconds. The results of sensitivity analysis, as well as average increase of solidification time in the case of increase of given parameter's value with value are shown for each case. The following observation can be accomplished on the basis of results placed in table 7: average increase of solidification time after adjustment of ranges of initial parameters' ranges, is very similar for all parameters. This situation takes place in both cases, where one second changes and two second changes were assumed. In the case, where changes of solidification time were assumed on the level of ten seconds, the values of changes for Brody's-Flemmings coefficient remained on the level close to changes that occur for two seconds variant. It is not surprising considering problem presented above. Due to the fact that range of coefficient remain unchanged (in relation to two seconds variant), it can be expected that changes caused by this coefficient will be equal to two seconds. Table 7 shows also the result of sensitivity analysis with Morris' method for such differentiated ranges.

The results of sensitivity analysis has not change regardless of assumed version. Additionally, variation ranges are characterized by significant differentiation (from ±0,092% for density of casting material, up to ±42% for Brody's-Flemmings coefficient). It can be observed on the basis on table 4. Obviously ranges increased, in the case of assuming higher increase of solidification time. Proportion between these ranges has not change both for the case of increase of solidification time by two seconds (table 5), and by ten seconds (table 6). This enables formulating of additional conclusion – results of sensitivity analysis obtained with the use of Morris method considering modified sensitivity coefficient, are repeatable for different versions of determination of ranges of studied parameters' variation.

SUMMARY

This article presents the way of usage of sensitivity methods for determination such ranges of acceptable parameters' changes that will cause assumed changes of result value. There is no necessity to execute additional simulations with use of the model in presented way, as well as no necessity for carrying out additional complicated calculations. Although proposed formula is very simple, it enables to achieve satisfactory results. Presented solution It is possible to applicate presented solution just after suitable sensitivity analysis, basing on the results necessary to execute analysis. This is because no additional changes in the method of sensitivity analysis are required.

REFERENCES

Campolongo F., Braddock R., 1999, The use of graph theory in the sensitivity analysis of the model output: a second order screening method, *Reliability Engineering and System Safety*, 64, 1-12

Morris, M. D., 1991, Factorial Sampling Plans for Preliminary Computational Experiments, *Technometrics*, 33, 161-174.

Saltelli A., Tarantola S., Campologno F., Ratto M., 2004, *Sensitivity analysis in practice: a guide to assessing scientific models*, John Wiley & Sons, Chichester.

Sczygiol N., 2000, *Numerical modeling of thermo-mechanical phenomena in a solidifying casting and a mould*, Publishing House of Czestochowa University of, Czestochowa.

Sczygiol N., Dyja R., 2007, Evaluating the influence of selected parameters on sensitivity of a numerical model of solidification, *Archives of Foundry Engineering*, 7, 159-164.

Sczygiol N., Szwarc G., 2001, Application of enthalpy formulation for numerical simulation of castings solidification, *Computer Assisted Mechanics and Engineering Sciences*, 8, 99-120.

Wood W. L., 1990, *Practical time-stepping schemes*, Clarendon Press, Oxford.

ZASTOSOWANIE METODY MORRISA DO OKREŚLENIA PRZEDZIAŁÓW ZMIENNOŚCI PARAMETRÓW POWODUJĄCYCH ZAŁOŻONE ZMIANY WYNIKÓW OBLICZEŃ

Streszczenie

W pracy przedstawiony jest sposób wykorzystania analizy wrażliwości do wyznaczenia dopuszczalnych przedziałów niepewności parametrów badanego modelu. Wykorzystywaną metodą jest metoda bazująca na metodzie Morrisa ze zmodyfikowanym wskaźnikiem wrażliwości. Badanym modelem jest solwer systemu NuscaS, który pozwala na przeprowadzanie symulacji krzepnięcia odlewów wykonanych ze stopów dwuskładnikowych. Model ten zbudowany jest w oparciu o metodę elementów skończonych, która wykorzystana jest do rozwiązania równania przewodzenia ciepła. Badany model wykorzystuje sformułowanie entalpowe do uwzględnienia zjawisk związanych z krzepnięciem. Dopuszczalne przedziały niepewności parametrów wyznaczane są w taki sposób, aby przyrosty wartości parametrów powodowały założone uprzednio zmiany wielkości wynikowej.

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