



ABILITY OF MATHEMATICAL MODELLING IN EXPLAINING REAL CASTING STRUCTURES

NOTWENDIGKEIT FÜR MATHEMATISCHE MODELLIERUNG DER GEFÜGEBILDUNG IN DEM GUSSTÜCK

НЕОБХОДИМОСТЬ МАТЕМАТИЧЕСКОГО МОДЕЛИРОВАНИЯ ФОРМИРОВАНИЯ СТРУКТУРЫ ОТЛИВОК

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Abstract: The high requirements for the materials utilized in machine engineering impose fundamental knowledge of the new phase formation processes in casting. The paper highlights the role of the phase formation basic kinetic equation for the mathematical modeling of the structures produced by casting. The casting process is presented on the example of Stefan's three dimensional problem for solidification of casting for copying machine drum. The relation is indicated between Stefan's type of problems and the phase formation basic kinetic equation for casting structures description.

KEYWORDS: mathematical modeling; Stefan's problem; phase formation; structures of cast materials and castings.

1. Introduction

Foundry is an important economic branch because structure formation processes suggest variety of possibilities for production of materials with the required for the practice operational properties - manufacture of parts with sophisticated geometry at minimum energy consumption. Foundry possesses a high potential for nature friendly technologies through energy and materials effectiveness with restoration of raw materials. In the process of developing new technologies an inter-disciplinary research approach is required such as the one developed in publication [1]. The major notion is: **Industry demands – effectiveness of energy and materials → foundry → machine design → material science + metal science → basic processes → operational properties of cast materials and castings.**

On the basis of Balevsky - Dimov gas counter pressure casting method [7] the Institute of Metal Science at the Bulgarian Academy of Sciences, Sofia, develops casting machines [8,9,10,11,12,13,14]. Fig.1 presents a general view of gas counter pressure pneumatic machine:



fig.1, General view of machine – type VP 1000

The new casting machines provide high operational properties for the materials and castings.

In addition to that the IMS-BAS carries out researches for production of metal powders [15] and metal glasses [16].

Fig.2 presents castings and parts developed in: IMS-BAS, in plants in the

country and abroad –

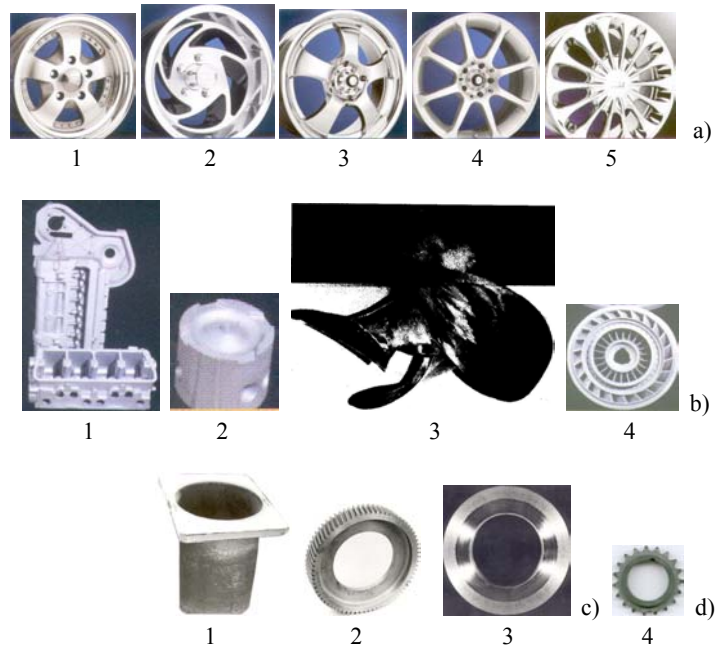


fig.2, a) 1÷5 – automobile wheels cast by gas counter pressure; b) – parts for internal combustion engines 1 cast by gas counter pressure, part 2 cast by squeeze casting method, 3 – propeller cast by gas counter pressure, 4 – pump turbine wheel cast by gas counter pressure; c) centrifugal casting 1 – cast for buffers, 2 – cog wheel, 3 – bimetallic casting; d) – powder metallurgy - cog wheel

The paper presents the role and place of the phase formation kinetic equation for mathematical modeling of the new structures in the casting process.

2. Methods and conditions for resolving the problem

2.1 Three-dimensional mathematical model of solidification–Stefan's problem and finite elements method

It is well known that the classical mathematical theory of casting is Stefan's problem [5] of general form (1÷1.3): heat conductivity equation for the area Ω with boundary Γ (see fig.4):

$$c_{EF} \rho \partial_t T = \lambda \partial_{xx} T + \lambda \partial_{yy} T + \lambda \partial_{zz} T \text{ in } \Omega, \quad (1)$$

$$\text{at initial condition for } t = 0, \quad T(x, y, z) = \text{const} \quad (1.1)$$

$$\text{and boundary conditions for } t \geq 0 \text{ at the boundary } \Gamma, \quad \lambda \partial_n T = \alpha [T_0 - T_w], \quad (1.2)$$

where T is temperature, t - time, λ - heat conductivity, ρ - density, c - thermal capacity; n is a normal to Γ , α - coefficient of convective heat transfer, T_w - environmental temperature; In the two phase area the effective value of

melt thermal capacity $c_{ef} = c + d_T S_F(T)$ is determined, where S_F is a function of Gauss type.

Having in view step solving of the temperature problem, the derivative of T by time is presented as

$$\partial_t T = \frac{T - T_0}{\Delta t}, \quad (1.3)$$

where T_0 is the temperature at the beginning of the step, and Δt - duration of the step in time.

After application of Galerkin's method and finite elements method accounting for (1.1) ÷ (1.3), the differential equation (1) is transformed into a system of algebraic equations.

We apply the described mathematical model for numerical experimentation of the solidification process of the casting (alloy A7) of which, after machining, the part shown in Fig. 3 is produced:

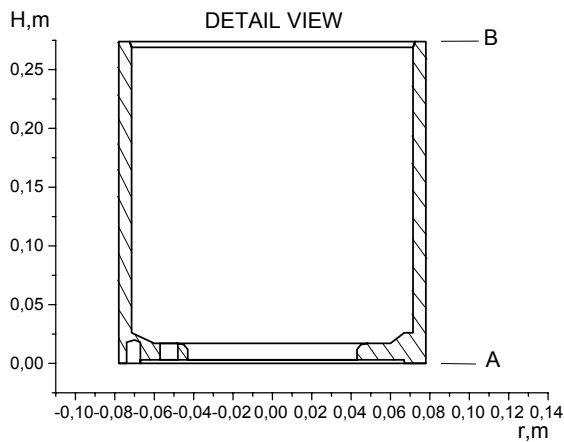


fig.3, Copying machine drum of high class of smoothness and accuracy on which operation coating is applied; The problem is divided into two: 1. Problem of casting solidification; 2. Problem of casting die non-stationary temperature field. Each of the two problems is solved independently and the connection between them is performed by the coefficient of surface convective heat transfer between the casting and die (see fig.4). At each step both problems are solved in succession changing the boundary condition (1.2). When the first problem is solved (for the casting) we assume that T_0 designates the temperatures of the casting boundary points and T_w - the temperatures of the die boundary points. When solving

the second problem we assume reversibly that T_0 designates the temperatures of the die boundary points and T_w - the temperatures of the casting boundary points.

Fig. 4 shows the general diagram of the casting-die system.

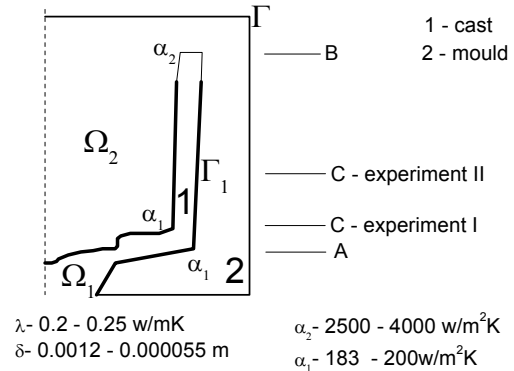


fig.4, cross-section of the symmetric system: 1 casting Ω_1 (with boundary Γ_1) - 2 die Ω_2 (with boundary Γ_1 and Γ); λ - heat conductivity coefficient of the coating of the die operational surface; δ - coating thickness; α_1 and α_2 - heat transfer coefficient on the die operational surface defined as λ/δ

It is well known that the basic requirements for every casting are: absence of shrinkage and the porosity has to be negligible. These defects are removed by providing a good feeding with melt of all the parts of the casting. In numerical simulation particular attention is paid to the part of the integration zone between the planes A and B (fig. 3 and fig. 4).

The effect of coating (created in IMS-BAS [18,19,20]) on the solidification process is studied by two types of numerical experiments with no accounting for the filling. It is assumed for the first of them a constant value for the coefficient of heat transfer between the casting and the die 1 - $\alpha = \text{const} = 2000 \text{ w/m}^2 \text{ K}$, and for the second - the heat transfer coefficient is a function of the height z 2 - $\alpha = f(z)$ (see fig. 4).

The results obtained for both types of numerical experiments are presented by: 1. temperature gradient of the average temperatures in the cross-sections along the height H of the casting from A to B; 2. temperature gradient along the radius r for cross-section C between A and B. The cross-section C is the last one where we have crystallization after certain moment of the crystallization process.

It is well known that the temperature field of the solidifying casting is the major carrier of information about the occurrence of the above said defects. Fig.5 presents the casting temperature gradients along the height and fig.6 fig.7 shows the temperature distributions along r : for experiment 1 - $\alpha = \text{const} = 2000 \text{ w/m}^2 \text{ K}$, and experiment 2 - $\alpha = f(z)$. Data about the average temperatures in the cross-sections from A to B - in fig.5: for the moment 7th second of experiment "I" and for 43rd second of experiment "II".

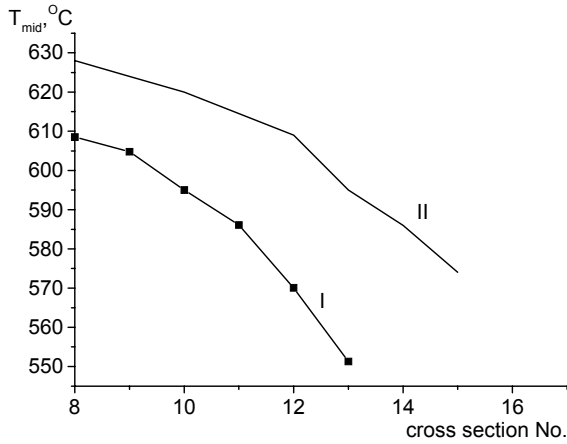


fig. 5, average temperature variations in cross-section along the casting height obtained in two numerical experiments: I – numerical experiment with constant heat transfer coefficient $\alpha(\lambda_{06}/\delta_{06})=2000\text{w/m}^2\text{K}$ for $t=7\text{sec}$; II – numerical experiment with different heat transfer coefficients $\alpha_1[(\lambda_{06}/\delta_{06}(z))]$ and $\alpha_2[(\lambda_{06}/\delta_{06}(z))]$ for $t=43\text{sec}$. The effect of heat transfer coefficients α_1 and α_2 on the temperature distributions along r are presented in fig. 6 for cross-section A:

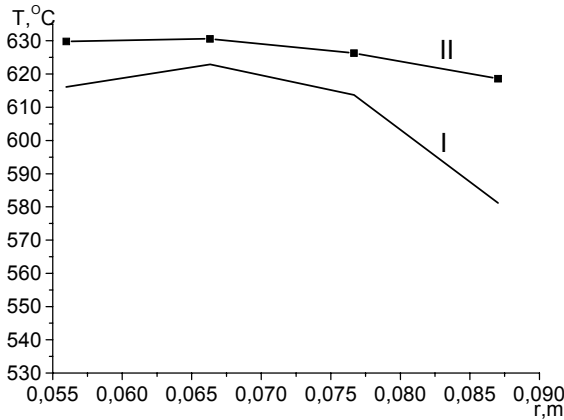


fig. 6, temperature distribution along r in the casting - cross-section - A, for experiment I and II

The difference between the temperature distributions along r is considerable in both types of experiments. In experiment I the whole cross-section is in the two-phase crystallization area with temperature difference $\sim 30\text{K}$ between the maximum and minimum temperatures. In experiment II a much more favorable temperature distribution is obtained, as temperature difference $\sim 10\text{K}$ and only the most outer part of the cross-section has crystallized. More favorable conditions are achieved for feeding the casting in the respective cross-section A.

Fig. 7 presents the temperature distributions along r in the last cross-section where there is crystallization – that is cross-section C (I experiment and II experiment):

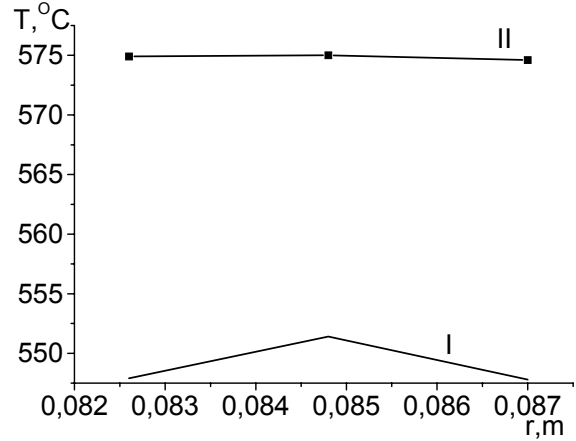


fig. 7, temperature distribution along r in the casting, in cross-section C, where there is crystallization for: experiment I and experiment II

Here the difference is even greater compared to the results in fig. 6. It is obvious that in the second type of experiments the possibility for feeding the casting is much better.

In experiment I (fig. 5, 6 and 7) the casting crystallizes between 22nd u 23rd seconds and the end of crystallization in experiment II is around 124th second.

The most general conclusion of the performed numerical experiments is that the effect of the coating on the crystallization process is significant and it can be used as an important local parameter for development of casting technology.

In accordance with the casting criteria there is a great possibility for porosity in experiment I, while the more favorable temperature gradients along z and r of the casting decrease the probability to produce porosity II (fig. 4, 5, 6 and 7). These results, as we have mentioned, do not determine the complete technology although they are sufficient for our work.

It is well known that the structure of the cast materials and castings is a carrier of their operational properties [1,2,3,4,5,6], but it is also known that in the frames of the mathematical model of solidification there is no possibility for evaluation of the structure formation processes.

2.2 Phase-formation basic kinetic equation

Publications [6,3] have developed a detailed mathematical model of phase transition of first order on the basis of phase formation basic kinetic equation formulated by D. Kashchiev and N. Miloshev's results for its solution. The general form of the basic kinetic equation for the case of variable oversaturation $\Delta\mu(t)$ [3] is:

$$\dot{Z}_n(t) = \sum_{m=1}^M [f_{mn}(t) - f_{nm}(t)] + K_n(t) - L_n(t), \quad (2)$$

where $Z_n(t)$ - function defining the number of complexes of n atoms in moment t , assuming that n -atomic complex has **equilibrium form**; $M(t)$ – the total number of atoms in the system in the moment t ; $f_{mn}(t)$ and $f_{nm}(t)$ - transient frequencies of aggregation and separation of parts of complexes with m and n

number of atoms ($m < n$); $K_n(t)$ and $L_n(t)$ - transient frequencies, at which the n -atomic complexes appear in/or disappear from the system as a result of non-aggregation processes. With suitably defined models of transient frequencies equation (2) is valid only for the initial stage of nucleation, but it permits description of the kinetics of nucleation and coagulation from an integrated point of view. Publication [3] considers in details the mathematical principles of modeling phase transition of first order for the case of casting. For Scillard's model ("bimolecular reactions" between monomers and complexes) N. Miloshev's results reveal great possibilities for mathematical modeling as the system (2) takes the following form:

$$\begin{aligned} \dot{Z}_n(t) = f_n(t)Z_n(t) - \bar{f}_n(t)Z_n(t) - \\ f_n(t)Z_n(t) + \bar{f}_{n+1}(t)Z_{n+1}(t), \end{aligned} \quad (3)$$

where $f_n(t)$ and $\bar{f}_n(t)$ - transient frequencies of aggregation and separation of monomers of n -atomic complexes.

2.3 Combined utilization of Stefan's three dimensional problem and the phase formation basic kinetic equation
The mathematical model of phase transition of first order [5] is based on the combined utilization of equation (1) and (3) by correlation scale for the two phase crystallization of the type:

$$\Delta V = L^3 = \left[\frac{D\Delta\mu}{GR} \right]^{1/2}, \quad (4)$$

where ΔV - characteristic local volume with edge L ; D - coefficient of self-diffusion in liquid phase; $\Delta\mu$ - thermodynamic motive force of the phase transition of first order; G - temperature gradient in ΔV . The rate of motion of the interface boundary is indicated by $R = \dot{X}g$, where \dot{X} - cooling rate and g - temperature gradient from the side of the solid phase. In equation (4) time participates through D , and in foundry, local solidification time t_f of certain volume is known, which is used in [3,5,6]. Thus for the local characteristic volume ΔV a generalized correlation coefficient B is introduced for defining t_f of the type [5]:

$$B = \frac{(\delta l_{CR})}{L} < 0.25 \Rightarrow \tau_B = \frac{B(\delta l_{CR})^2}{a} \pi t_f, \quad (5)$$

τ_B - time for the crystallization front shift at distance (δl_{CR}) in direction of the normal n ; a - coefficient of temperature conductivity. Equations (4) and (5) help to bind e.g. (1) and (3), the temperature field of the Stefan's three-dimensional problem of the two-phase zone allowing to connect the phase formation kinetics with the thermodynamic system deviation from equilibrium - $\Delta\mu$ and the nucleation work $W_n(\Delta\mu)$ [3,5]:

$$\Delta\mu = Q_L \ln \frac{T_L}{T}, \quad (6.1)$$

$$W_n(\Delta\mu) = -n\Delta\mu + S_n[\Delta\mu, \Phi(\theta)], \quad (6.2)$$

$$\Phi(\theta) = \frac{1}{4}(2 + \cos\theta)(1 - \cos\theta)^2, \quad (6.3)$$

where $T \in [T_L, T_S]$ - temperature interval of the two phase zone, T_L, T_S - temperature liquidus and solidus, Q_L - heat of phase transition; S_n - surface energy of the new phase nucleus; $\Phi(\theta)$ - function of angle θ of the pad wetting.

Equations (6) are common for the theory and working with them is comparatively easy, e.g. [17]: in case the wetting angle is $\theta=0^\circ \Rightarrow \Phi=0$ - complete wetting and no barrier for nucleation; in the case - $\theta \in [10^\circ \div 170^\circ] \Rightarrow \Phi \in [0,00017 \div 0,9998]$ - heterogeneous nucleation and finally - no wetting at $\theta=180^\circ \Rightarrow \Phi=1$ - homogeneous nucleation.

3. Possibility for mathematical modeling of structure formation processes by the phase formation basic kinematics equation

It is well known that eq.(6) are connected with the transient frequencies $[f_{mn}(t), \bar{f}_{mn}(t)]$ or $[f_n(t), \bar{f}_n(t)]$ i.e. eq.(6) are also the direct connection between Stefan's three dimensional temperature problem and the phase formation basic kinetic equation (3), which presents the kinetics of the new phase formation process.

Equations (4) and (5) allow that the casting volume and solidification time are presented as a sum of local volumes and local solidification times [2]:

$$\Omega_1 = \sum_{i=1}^{I_{MAX}} \Delta V_i; t_{CR} = \sum_{i=1}^{I_{MAX}} t_{fi}, \quad (7)$$

where I_{MAX} - maximum number of local volumes with their local solidification times. Then for $\forall (\Delta V_i \text{ and } \tau \in [0, t_{fi}])$ the results of the solution of eq.(3) are presented by the following equations [3]:

equation for nucleation rate $I_n(\tau)$ of complexes of n -atoms

$$I_n(\tau) = f_n(\tau)Z_n(\tau) - \bar{f}_{n+1}(\tau)Z_{n+1}(\tau), \quad (7.1)$$

equation for nucleation rate $X_n(\tau)$ of complexes with sizes greater than those of n -atoms

$$I_n(\tau) = X_n(\tau) \quad \forall n \in [1, M], \quad (7.2)$$

where eq. (7.2) - **the most general for the critical and above critical size**; $X_n(\tau)$ - total number of complexes with dimensions greater than n -atoms and it is presented by the expression

$$X_n(\tau) = \sum_{i=n+1}^M Z_i(\tau). \quad (7.3)$$

For the complex sizes in the total distribution eq.(7.3) it should be known that the number of atoms in the complex is $n(\tau) \phi \phi 1$ and only then work is possible, and with its effective radius $r_{ef}(\tau)$, which is an important geometric dimension connected with the structure of the new phase. Furthermore eq.(7.3) allows determination also of the maximum number N_m of the complexes in the local volume [3]:

$$N(\tau) = \int_{n(\tau)}^M X_n(\tau) dn \text{ and } \tau \rightarrow t_f \Leftrightarrow N_m = N_{MAX} \quad (7.4)$$

i.e. the maximum number of the grains in the local volume ΔV_i at $\tau = t_f$.

Equations (7) present in summary the possibilities for mathematical modeling of the structure formation processes in the solidification process during casting. For adequacy of a mathematical model through eq.(7) it is necessary to compare the rates of the two processes eq.(7.1) and eq.(7.2), that run in parallel. For instance:

the rate $I_n(\tau)$ is related mainly with appearance of new complexes (here clusters are included – complexes of

under critical dimensions); while the rate $\mathcal{X}_n(\tau)$ is connected not only with the nucleation of complexes with dimensions larger than n -atoms but also with the growth of the nuclei. Besides the effective radius of the complexes at the end of the crystallization in the local volume we also obtain direct connection with the average statistic geometric factor, as the mean grain diameter d_m of the polycrystalline structure is. That will determine the grain sizes in the different casting zones [17]. The correlation of the grain size in the individual zones determines the type of the structure: a) the most fine (fine grain); b) columnar crystals; c) equiaxed crystals as well as the final axial porosity.

All the above said we generalize under the schemes in accordance with [1,2] by one basic requirement: the crystallization in each local volume ΔV_i should follow the solidification in experiment II. In order to provide stable stochastic behavior of the solidification process it is necessary to observe the generalized principle of control [1] and to build the controllability operator of the open physical (thermodynamic) system [1,2] with parameters: input observable quantities – initial temperature of the

casting T_C^0 ; initial temperature of the die T_m^0 ; heat transfer coefficient of the die operational surface

$\alpha(z) = \frac{\lambda_{CV}}{\delta_{CV}(z)}$. The basic physical quantities for the process are the non stationary distribution of the average

temperatures along the casting height $\bar{T}(z, t)$ (fig.5);

the non stationary temperature distribution $\bar{T}_A(r, t)$ in cross-section A (fig.6); the non stationary temperature

distribution $\bar{T}(r_C, t)$ in cross-section C (fig.7). For the whole casting we introduce average quantities for the basic process – phase transition of first order: the

thermodynamic driving force $\Delta\bar{\mu}$; the nucleation work

$\Delta\bar{W}_n$; the nucleation rate $\bar{I}_n(\tau)$; the nucleation rate

$\mathcal{X}_n(\tau)$; the law of nuclei effective radius growth \mathcal{R}_{EF} ;

the grain mean diameter \bar{d}_m of the polycrystalline

structure. The outcome observable quantities in the case are: temperature distribution on the casting surface at the end of the

process $T_C(\Gamma_1, t_{END})$; temperature distribution on the die

surface at the end of the process $T_M(\Gamma, t_{END})$; grain mean

diameter for the whole casting $\bar{d}_m(x, y, z)$. The permissible

deviations of the major physical quantities in the controllability operator we indicate by δ . Then the general form of the controllability operator [1,2] is:

$$\mathcal{Y} = \begin{pmatrix} \bar{T}(z, t) & \bar{T}_A(r, t) & \bar{T}(r_C, t) \\ \Delta\bar{\mu} & \bar{W}_n & \bar{I}_n \\ \mathcal{X}_n & \mathcal{R}_{EF} & \bar{N}_m \end{pmatrix} \begin{pmatrix} T_C(\Gamma_1, t_{END}) \\ T_M(\Gamma, t_{END}) \\ \bar{d}_m(x, y, z) \end{pmatrix} + \begin{pmatrix} \delta\bar{T}(z, t) & \delta\bar{T}_A(r, t) & \delta\bar{T}(r_C, t) \\ \delta\Delta\bar{\mu} & \delta\bar{W}_n & \delta\bar{I}_n \\ \delta\mathcal{X}_n & \delta\mathcal{R}_{EF} & \delta\bar{N}_m \end{pmatrix} \begin{pmatrix} T_C^0 \\ T_m^0 \\ \alpha = \frac{\lambda_{CV}}{\delta_{CV}(z)} \end{pmatrix} \quad (8)$$

The main purpose is realization of structure homogenization in the casting that is presented in fig.8:

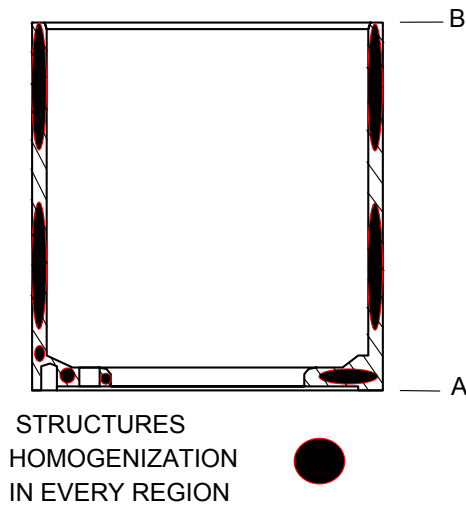


fig.8, regions of grain mean diameter observation and control $\bar{d}_m(x, y, z)$

Finally we fill the theoretical block diagram to create a strategy for control according to the variable parameters of controllability operator [1,2]:

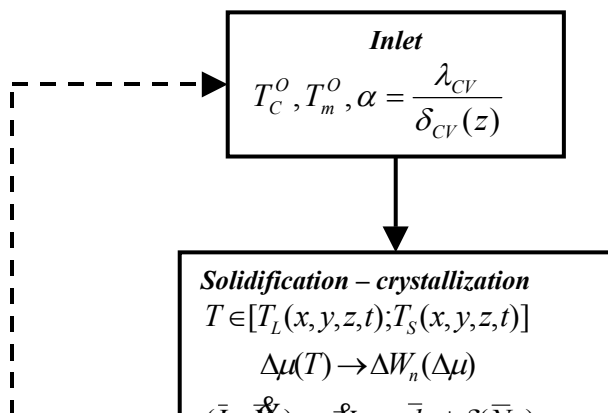


Fig.9, block diagram for assessment of control strategy; - the dashed line is the controlling effect (generation of an iteration) Finally it could be said that we have presented a most general strategy of the possibilities for mathematical modeling of the structure of castings and cast materials.

4. Conclusion

1. The heat transfer coefficient of the coating together with its thickness is a significant local parameter to create an **initial resistance** of the die operational surface during casting. In the particular example the coating affects the complete solidification process because the product is thermo-technically thin.
2. There is presented the fundamental connection for the joint utilization of Stefan's problem and the phase formation basic kinetic equation.
3. For every local volume the effective radius of the nucleation complexes in the end of the crystallization is also a direct connection with the grain mean diameter d_m of the polycrystalline structure. A basic average statistic geometric parameter generalizing the results of the casting process.
4. The phase formation basic kinetic equation transforms into a basic equation for mathematical modeling of the structure formation processes in casting. That is due to the fact that it presents the basic process – phase transition of first order.
5. We have developed a general methodological scheme for physical and mathematical modeling of the solidification and phase formation processes during casting.
6. The clear presentation of the structure formation processes together with the modern casting machines transforms foundry in a major branch of machine engineering.
7. Foundry is becoming a field of application of new investigation methods in the creation of new products of material science.

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