«Системні технології» 6 (125) 2019 «System technologies»
DOI 10.34185/1562-9945-6-125-2019-09
UDC 004.942:622.647.8 (043.3)

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SYSTEM ANALYSIS OF POROSITY FORMATION PROCESSES IN STEEL CASTINGS AND THEIR MATHEMATICAL MODELS

Annotation. The analysis of scientific and technical information about the hardening features of steel castings, which lead to the formation of shrinkage defects is presented. The mechanisms of the relationship of the casting properties of alloys are shown. The analysis of factors that determine fluidity is carried out. The technological parameters of casting are determined, which lead to the formation of pores in steel castings. The mechanisms of porosity formation of endogenous and exogenous nature are considered. Siverts law is given, that describes the dependence of gas concentration on pressure. Graphs of changes in the concentration of nitrogen and hydrogen in the pressure range 1 - 4 atm are given for medium alloyed steel, open-hearth steel, cast iron. The mechanism of the influence of temperature and gas pressure on the process of gas evolution in the melt is analyzed. Technological methods for influencing the solubility of gases during the solidification of the casting are described. The microporosity model of Advanced Porosity Module, the Niyama criterion are analyzed. The need for further studies to develop a general model for the formation of shrinkage defects, which will take into account, inter alia, the dependence of the concentration of gases dissolved in the metal on pressure temperature, is noted.

Keyword: shrinkage, defects, porosity, castings, steel, casting properties, fluidity, impact, melt, Siverts law, gas concentration, pressure, Niyama criterion, complex mathematical model.

Introduction. It is known that mechanical engineering invariably occupies one of the leading places in the structure of goods manufacture of all industrially developed countries of the world. In particular, in 2017 in Ukraine, the share of sold engineering products in the total industrial volume amounted to 10.9% [1]. At the same time, the importance of the role of the metallurgical and foundry manufacturing as the main procurement bases for engineering remains at a high level and, along with this, the requirements for the quality of ingots and castings are increasing. The heterogeneity of the size, shape and distribution of crystals in the volume of the cast billet, porosity, and chemical heterogeneity are the main problems in obtaining high-quality castings or ingots, despite the complex of specific thermophysical

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conditions for the formation of the structure and geometric characteristics, due, in turn, to technological features of manufacturing [2, 3]. A feature of such technological schemes is, first of all, the mandatory availability of additional rather sophisticated equipment, which entails a rise in the cost of the process of developing new technologies and improving existing ones. In this regard, there is an urgent need to develop new mathematical models for evaluating parameters technology without additional computational experiments. Therefore, the increasing attention of scientists and practitioners is attracting questions related to the improvement of existing and the development of new mathematical models that provide an adequate description of the processes that occur in castings during solidification in a mold. In this case, the models of porosity formation under conditions of external influence on the melt in the mold are of the greatest relevance [4, 5].

Method. To determine the cause or probable sources of gas porosity in the castings, one should pay attention to the nature of the pores formed. If porosity rarely appears in one or more castings from a given melt, this indicates that the cause of the defect is associated with imperfections in the shape design. If all castings are affected by shells, then the defect is caused by the poor quality of the metal, namely gas saturation, which affects the basic casting properties of metals and alloys that determine their manufacturability, namely the suitability for obtaining castings from them of the required configuration with high operational properties, given dimensional accuracy and required surface quality [6].

Foundry properties appear both in melts and at all stages of their solidification and cooling. The most important casting properties of alloys (Figure 1) include fluidity, shrinkage, a tendency to segregate, as well as a tendency to form non-metallic inclusions, to absorption of gases, the formation of internal stresses and internal cracks [6, 7].

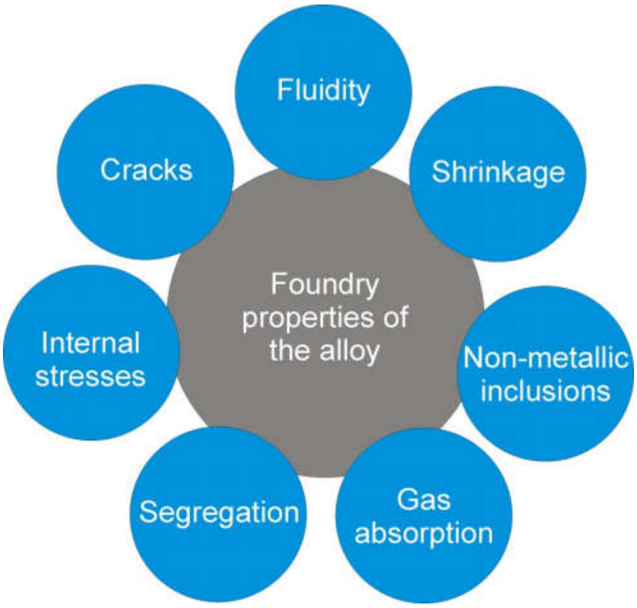

Figure 1 – Foundry properties of alloys

One of the main technological properties of liquid alloy in foundry is fluidity [7]. With low fluidity, the movement of the melt in the mold may cease before it is full. This is most likely in the manufacture of large thin-walled castings, especially if the alloy in the mold cools quickly (for example, when casting in metal or raw sand forms). Fluid flow affects the fillability of the form with the melt, the clarity of the reproduction of the relief of the mold cavity.

The fluidity is influenced by many factors related to the properties, state and structure of the melt (figure 2):

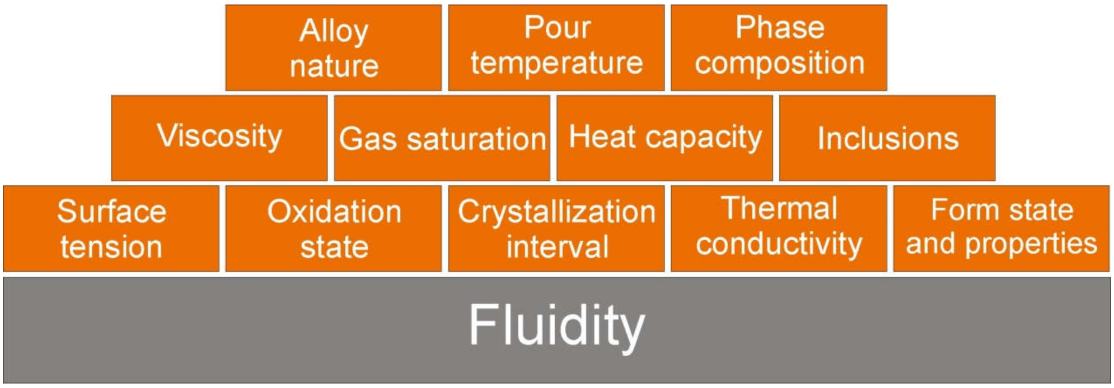

Figure 2 - Factors that affect the fluidity of alloys

Alloys that harden with the formation of a eutectic have higher fluidity [7]. In steel and cast iron, fluidity decreases with increasing sulfur content and increases with increasing phosphorus and silicon content (Figure 3). Overheating of the alloy increases its fluidity.

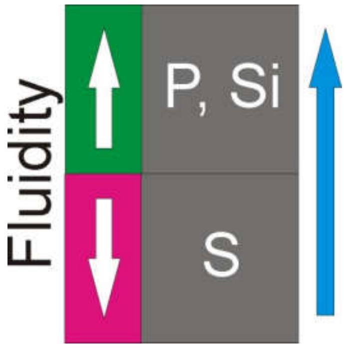

Figure 3 - An example of factors affecting the fluidity of Fe-C alloys

One of the conditions for obtaining a high-quality casting is to ensure smooth filling of the mold with minimal turbulence of the melt flow at the beginning of casting and a favorable distribution of flow rates in the gating system and form, which allows to reduce the oxidation and secondary gas saturation of the melt [8]. The turbulence of the melt flow in the form, first of all, depends on the melt pouring rate (table 1).

Table 1

The impact of the speed and nature of filling the form on the defect's formation in the casting

Fill Speed / Character	Impact on the casting properties of alloys	Defect
Slow / smooth	- oxidation - gas saturation	- underfilling - junctions - subcortical shells
Pulsating	- flow continuity - discharge	- destruction of form - contamination of the surface layer of the casting - burnout
Fast		- formation of shells - air capture

An increase in the speed of the melt when filling thin-walled castings leads to disruption of the flow continuity, air capture, and the formation of endogenous shells. If the casting speed is insufficient, defects occur in the castings associated with the crystallization process - junctions, uningots, inversions, etc.

Ensuring the optimal hydrodynamic and thermal parameters of the technological process plays a decisive role in obtaining castings with the required level of physical, mechanical and operational properties [6].

The presence of gases in metals and alloys has a great influence on the casting, physic-mechanical and operational properties of cast parts. The source of gases in metals can be:

- charge materials,
- atmosphere of the melting unit,
- blast supplied to the surface or deep into the molten bath (technical oxygen, air, other gases),
- ferroalloys introduced into metal or slag during the process of melting and casting,
- refining and modifying additives,
- gases generated by the combustion of fuel.

The permissible limits for the content of gases and non-metallic inclusions for various alloys are determined by the relevant standards.

Gases are present in the metal in:

- free state in pores and shells,
- solid chemical compounds with elements that make up the alloy (oxides, nitrides, hydrides),
- a dissolved state in liquid and solid solutions, thin layers adsorbed on various structural components of the metal matrix.

The dissolution of gases in metals depends on the nature of the gases, the state of metals and alloys, and ceteris paribus on the temperature and partial pressure of gases. The dissolution of gases is an endothermic process. The release of gases in the free state occurs as a result of a decrease in their solubility in the melt and solid phase at lower temperatures. With increasing temperature of the metal, depending on the change in enthalpy, the solubility of gases can increase or decrease.

In the case of the dissolution of diatomic gases in pure iron, there is a relationship between the partial pressure of these gases in the atmosphere above the melt and the solubility of the gas in the metal. The dependence of the concentration of substance C from acting pressure p, Siverts law or square root law [7]:

$$C = C_0\sqrt{p/p_0}\,, \qquad (1)$$

where C_0 – substance concentration in balance with standard pressure p_0.

The law is valid in cases where the diatomic gas adsorbed by a metal first dissociates into two atoms that dissolve to form a solution or chemical compound [7]. If, when hydrogen or nitrogen is dissolved in a metal, compounds containing more than one gas atom are formed (e.g., ZrH_2, TiH_2, SiH_4, etc.), the square root law is not valid. In the process of melting iron-carbon alloys, the metal does not contain a significant amount of hydride or nitride-forming impurities, therefore, the square root law for hydrogen and nitrogen is satisfied.

Also, the additives introduced during the melting process (lime, ore, ferroalloys, etc.) also influence the gas content in the metal.

Steel scrap usually contains 0.0004–0.0008% H and 0.003–0.005% N, the oxygen content depends on its chemical composition, as well as on the degree of oxidation of the surface, a lot of hydrogen is also added with rusty scrap [8, 9]. The ingress of about 1% rust into the melting unit together with the charge leads to an increase in the hydrogen content of about 2.5 m^3 per 1 ton of steel. Ferroalloys such as ferromanganese and ferrosilicon are difficult to liberate from hydrogen even during high-temperature calcination. Ferrosilicon at a temperature of 1000 °C can contain up to 6 · 10–5 m^3/100 g of hydrogen, and ferromanganese up to 3 · 10–5 m^3/100 g, nickel and chromium - 0.8 and 0.1–0.2 m^3/100 g, accordingly. The main source of the gaseous phase when casting in sandy-clay forms is water. In a thin surface layer of the shape of the vapor forms instantly: 1% moisture in this layer is enough for the amount of vapor to be approximately 2/3 of the volume of the metal. For example, in cast iron, gas adsorption can be observed on the surface of graphite inclusions.

The oxygen-converted medium alloy steel contains 0.002-0.005% N, the open-hearth steel - 0.004-0.008% N and the electric steel contains 0.006-0.012% N. Cast iron usually contains 0.0010-0.0025% H and about 0.005% N. The hydrogen content in cast iron in the case of high humidity during metal purging, as well as when natural gas is supplied to a blast furnace, can be significantly higher [7]. Figure 4 shows the dynamics of changes in gas concentration for some types of cast steels.

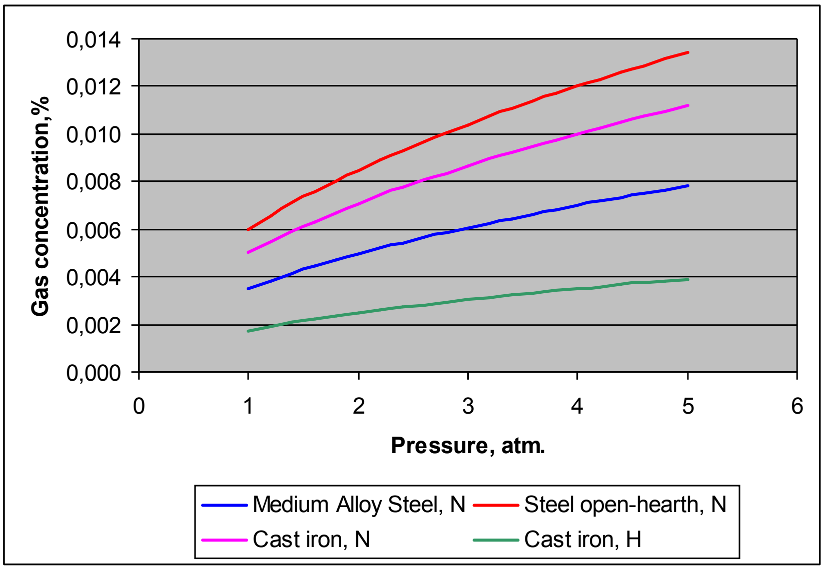

Figure 4 – An example of a change in the concentration of gases in the melt with increasing pressure (at a constant temperature)

To minimize the harmful effects of the increased content of hydrogen and nitrogen, pure charge materials are used in industrial practice, they are melted in an atmosphere with a minimum content of hydrogen and nitrogen, the metal is treated with vacuum, the metal is purged with inert gases, and pressure is applied during the solidification of the workpiece in the form [8, 9].

The mechanism of the influence of temperature and gas pressure on the process of gas evolution in the melt (figure 5).

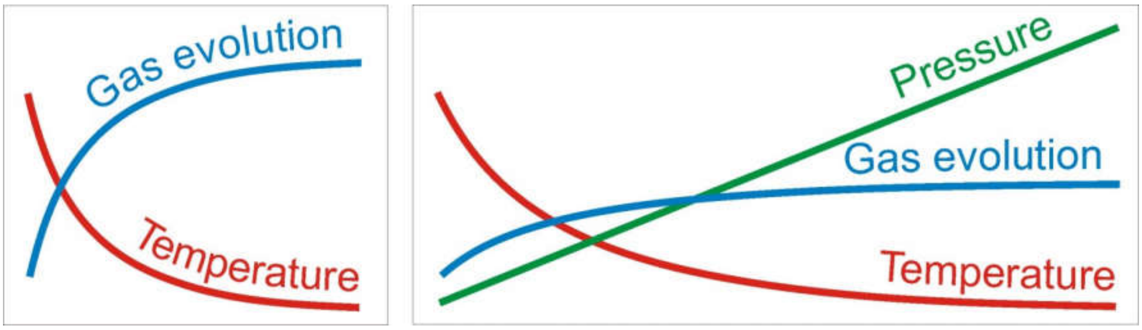

Figure 5 - Patterns of gas evolution in the melt during solidification

Oxygen forms oxides in the alloys, which belong to non-metallic inclusions. Regarding the oxygen content in steels, it can be said that a metal almost always contains less oxygen than under balance conditions with slag.

The transition of oxygen from the gas phase through the slag to the metal can occur as a result of direct contact of the oxidizing phase (O_2, CO_2, H_2O) with metall.

Oxygen is present in liquid steel in the form of solution or in the form of oxide non-metallic inclusions. With increasing melt temperature, the solubility of oxygen in liquid iron increases. A certain amount of gases dissolved in the metal during crystallization is released in the form of bubbles, some of which remain in the ingot. Nonmetallic inclusions can concentrate at the metal – gas bubble boundary [8, 9].

Due to the decrease in the solubility of gases with decreasing temperature, especially during the period of completion of the crystallization process, steel containing a large amount of gases is blistering, with low mechanical properties and is unsuitable for use. Elevated oxygen concentrations in mild steel can cause bubble formation due to reactions with carbon $[O] + [C] = CO_{gas}$.

The continuity of the alloy in the casting breaks when gas bubbles appear in the liquid or crystallizing alloy.

Shells of an endogenous nature arise due to the release of gases from the cooling melt. The formation of this type of shells can occur as a result of a decrease in the solubility of gases with a decrease in the temperature of the melt or due to chemical reactions, the product of which is the gas phase (for example, $FeO + C = Fe + CO$).

To form an independent phase in a liquid metal, a gas bubble must overcome atmospheric pressure, metallostatic pressure and surface tension of the melt. The formation of bubbles, like crystals in a liquid, occurs more easily on solid surfaces in the form of heterogeneous nuclei from fluctuations of dissolved gas atoms. If neutral gas bubbles are introduced into the melt, the partial pressure of ordinary gases in them will be zero, therefore, dissolved gases will easily penetrate into the bubble [8]. Bubbles either have time to appear on surface or not, and, as a result of this, a gas shell forms in the cast.

Bubbles, the formation of which occurs in the zone of oriented crystals, grow between them and have an elongated shape, called cellular bubbles [9]. At the boundaries of the columnar crystal zone, enhanced bubble formation is observed associated with a change in crystallization. In the middle part of the casting, the formation of liquidation bubbles, which do not have a certain orientation, occurs, as do the crystals surrounding them. The release of gas dissolved in the metal can easily occur in shrink shells and pores.

In order to prevent the formation of gas shells of an endogenous nature, measures are taken throughout the entire manufacturing process for the preparation of liquid metal, casting and crystallization of the casting; preparing the charge materials in order to reduce the degassing of the starting materials; accessible technological methods prevent the possibility of gas absorption during melting, the release of metal into the ladle and pouring it into molds [10].

For alloys that are particularly prone to gas absorption, they are melted in a protective atmosphere (vacuum, neutral or reducing atmosphere), the melt is protected by slags and fluxes, various refining additives are used that react with the gas dissolved in the metal to form non-metallic inclusions.

To degas the melt outside the melter, the melt is purged with gases, ultrasonic treatment and other methods of electrophysical effects on the metal are performed. In the manufacture of castings from light alloys, the crystallization method under an overpressure of 4–5 atm is particularly well recommended. The increase in the rate of solidification also acts in a similar way: as a result of a large temperature gradient over the cross section of the casting, gases having time to stand out from the melt can move to areas where defects of shrinkage origin are concentrated. Thus, when creating directional solidification, it is possible to withdraw the gas released from the melt into profit [10].

Results and discussion. In order to conduct a preliminary theoretical analysis of the gas saturation of melts, modern mathematical modeling systems offer a fairly large number of different programs. To record gas component in the gas evolution from liquid metal according to the Sieverts law, a special Advanced Porosity Module (APM) is used, which is based on solving the Darcy equation and microsegregation of gas, taking into account the pressure drop in the solid-liquid phase and gas evolution from the melt [11].

In order to accurately calculate the pressure drop in the solid-liquid zone, a dynamic cleaning technique is implemented: a fine and uniform finite-volume mesh is re-attached to the finite-element mesh used to calculate hydrodynamic and thermal problems. For each variable step, cells are activated that fall into the solid-liquid zone and control the formation of porosity only for this volume, with the corresponding boundary conditions [11, 12].

The microporosity model used by APM is based on two main phenomena - pressure drop in the solid-liquid zone and gas evolution from the melt. In this model, it is assumed that the motion of a liquid metal in a solid-liquid zone is controlled only by the pressure distribution. Local pressure consists of several components:

$$P_l = P_a + P_m + P_d\,, \tag{2}$$

where P_a – atmospheric or external pressure; P_m – metallostatic pressure; P_d – dynamic pressure responsible for the movement of fluid in a solid-liquid zone.

The velocity of the intradendritic fluid is determined from the Darcy equation:

$$V = -\frac{k}{\mu} grad\ P_d = -\frac{k}{\mu} grad\ P_l - P_l\, g\,, \tag{3}$$

where k – hard shell permeability; μ – dynamic fluid viscosity; P_l – local pressure; g – gravity vector.

Dynamic viscosity is calculated from the equation

$$\mu = \mu_0 \exp\left(\frac{E_\mu}{RT}\right), \qquad (4)$$

where μ_0 – viscosity at standard temperatures; E_μ – activation energy; R – universal gas constant.

APM takes into account the influence of some elements present in the alloy on the solubility of gases.

As applied to injection molding, gas evolution is possible only in the thermal components of the casting, the solidification of which occurs after the solidification of the feeder. It is also necessary to take into account that the solidification of the feeder in the casting occurs under excessive pressure, and gases from the metal can be released only at atmospheric pressure or below it. A certain amount of time is required to compensate for this excess pressure by shrinkage, which will lead to an even greater narrowing of the area of the Siverts law [13].

At the same time, APM module ignores the gas trapped by the metal when filling the mold cavity, while it is the main culprit in the formation of pores during injection molding. Gases in the form can affect the hydrodynamics of the process of movement of a metal stream, taking into account backpressure is especially important when modeling injection molding.

In injection molding, the porosity in most cases is mixed - gas is released from the metal into the pores of shrinkage origin, a significant part of the gas located in the mold cavity can mix into the liquid metal when filling.

Program of mathematical modeling of heat and mass transfer processes developed by FLOW SCIENCE INC (USA) is of great interest. The library of mathematical models includes solutions not only of the Navier-Stokes equations, but also of flows around solids of arbitrary configuration, solidification / melting taking into account the heat of phase transition, formation of gas bubbles, surface tension and adhesion to walls, application of external forces and pressures, etc.

To solve the problems of foundry and metallurgical production, the program allows you to simulate the processes of formation of shrinkage defects in the form of porosity (loosening) or shells, checking the possible formation of unsalts and uningots, analyzing the melt flow with air mixing and slag inclusions, filtering through ceramic filters, etc. [12 - 15].

The main disadvantage of the FLOW-3D program is that it uses an orthogonal coordinate system to solve problems. Complex geometric structures are described using volumetric bodies and thin walls using the fractional area / volume method (FAVOR).

A common approach for calculating porosity is the criteria approach.

Niyama et al. [16] established a criterion to determine the appearance of shrinkage porosities. Therefore they considered different porosity criterion which can be calculated easily and compared these values with experimental results. As a result a porosity criterion was investigated, which is now widely used and known as Niyama criterion. The criterion can be calculated with the following equation (5)

$$N_y = \frac{G}{\sqrt{\dot{T}}} < 1 \qquad (5)$$

where G is the thermal gradient and $\dot{T}$ is the cooling rate. Regarding steel, the critical value is around 1.0 [(K min)$^{0.5}$/cm]. A Niyama value below this critical value leads to the occurrence of shrinkage porosity. The advantage of this criterion is the independence of the casting geometry. Nevertheless, the critical value depends on the corresponding casting material and must be determined for every casting material [17].

The Niyama criterion was further developed by Carlson et al. [18]. The aim of this improvement was to predict not only the position of the shrinkage porosity in the casting, but also the amount of the pore volume fraction. The advanced Niyama criterion is also called the dimensionless Niyama criterion and can be calculated according to equation (6)

$$N_{y^*} = \frac{G\lambda_2\sqrt{\Delta P_{cr}}}{\sqrt{\mu_l \beta \Delta T_f \dot{T}}} = N_y \frac{\lambda_2\sqrt{\Delta P_{cr}}}{\sqrt{\mu_l \beta \Delta T_f}} = \sqrt{I\left(g_{l,cr}\right)} \qquad (6)$$

where λ_2 is the secondary dendrite arm space, ΔP_{cr} is the critical pressure drop; μ_l is the liquid dynamic viscosity; $\beta = (\rho_s - \rho_l)/\rho_l$ is the solidification shrinkage; $\Delta T_f = T_{liq} - T_{sol}$ is the freezing range and $I\left(g_{l,cr}\right)$ is an integral, which depends on the solid fraction-temperature curve. For simple curves the integral can be calculated analytically with equation (7)

$$I\left(g_{l,cr}\right) = \int_{g_{l,cr}}^{1} 180 \frac{\left(1-g_l\right)^2}{g_l^2} \frac{d\theta}{dg_l} dg_l \tag{7}$$

where $\theta = \left(T - T_{sol}\right) / \Delta T_f$ is the dimensionless temperature. Further details regarding the dimensionless Niyama criterion can be found in [18]. Carlson et al. use the dimensionless Niyama criterion to understand the formation of shrinkage porosity for an aluminium alloy, a magnesium alloy and mild steel.

A simple permeability model, which is widely used, was applied at these simulations. The Carmen-Kozeny model is an isotropic permeability model and based on the pressure drop during the flow of a fluid through a porous medium. Equation (8) describes this model.

$$K = K_0 \frac{g_l^3}{\left(1-g_l\right)^2} \tag{8}$$

K_0 represents the microstructure of the steel and can be calculated with $K_0 = \lambda_2^2 / 180$, λ_2 is the secondary dendrite arm space. For the calculation of the permeability a secondary dendrite arm space λ_2 of 50 µm was estimated.

Conclusion:

1. The analysis of the results of theoretical and practical research of the processes occurring in the alloy during solidification in the mold is given. The processes of the relationship of the casting properties of alloys and possible shrinkage defects are described.

2. The mechanisms of porosity formation of endogenous and exogenous nature are considered. Conclusions are made about the significant influence of the parameters of the process of pouring metal into the mold on the formation of porosity.

3. Using the Siverts law, the dependences of changes in the concentration of nitrogen and hydrogen in the pressure range 1–4 atm were obtained for some types of cast alloys. Technological methods of influence on the solubility of gases during the solidification of the casting are described.

4. The analysis of the mechanism of the influence of temperature and gas pressure on the process of gas evolution in the melt is made.

5. The mathematical model of Advanced Porosity Module for assessing microporosity and the Niyama criterion are analyzed. It is established that Advanced Porosity Module model is commercial in nature and has a closed mathematical apparatus. The Niyama criterion does not give a direct assessment of porosity, and also does not allow to correctly take into account the pressure change in the solidification zone of the casting, the dependence of the concentration of dissolved gases on temperature and pressure.

6. The necessity of developing mathematical models of porosity formation, which takes into account the dependence of the solubility of gases in the melt not only on pressure but also on temperature, has been established.

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Received 11.12.2019.
Accepted 13.12.2019.

Системний аналіз процесів утворення шпаристості в сталевих виливках і їх математичних моделей

Представлений аналіз науково-технічної інформації щодо особливостей затвердіння сталевих виливків, які призводять до утворення усадкових дефектів. Показані механізми взаємозв'язку ливарних властивостей сплавів. Проведено аналіз факторів, які визначають текучість. Визначено технологічні параметри заливки, які призводять до утворення пор в сталевих виливках. Розглянуто механізми утворення пористості ендогенного і екзогенного характеру. Наведений закон Сівертса, який описує залежність концентрації газів від тиску. Наведено графіки зміни концентрації азоту і водню в діапазоні тисків 1 – 4 атм. для середньолегованої стали, мартенівської сталі, чавуну. Проведено аналіз механізму впливу температури і газового тиску на процес виділення газу в розплаві. Описано технологічні прийоми впливу на розчинність газів в процесі затвердіння виливки. Проаналізовано модель мікропористості використовувана Advanced Porosity Module, критерій Niyama. Визначена необхідність подальших досліджень для розробки загальної моделі утворення усадкових дефектів, яка буде враховувати, в тому числі, залежність концентрації розчинених в металі газів від температури та тиску.

System analysis of porosity formation processes in steel castings and their mathematical models

The analysis of scientific and technical information about the hardening features of steel castings, which lead to the formation of shrinkage defects, is carried out. The mechanisms of the relationship of the casting properties of alloys are shown. Siverts law and graphs of changes in the concentration of nitrogen and hydrogen in the pressure range 1 - 4 atm are given for some types of cast alloys. The mechanism of the influence of temperature and gas pressure on the process of gas evolution in the melt is analyzed. We analyzed Advanced Porosity Module microporosity model, criterion Niyama.

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