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Carburizer particle dissolution in liquid cast iron – computer simulation

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Abstract

In the paper issue of dissolution of carburizing materials (anthracite, petroleum coke and graphite) particle in liquid metal and its computer simulation are presented. Relative movement rate of particle and liquid metal and thermophsical properties of carburizing materials (thermal conductivity coefficient, specific heat, thermal diffusivity, density) are taken into consideration in calculations. Calculations have been carried out in aspect of metal bath carburization in metallurgical furnaces.

Keywords: Cast iron, Carburization, Carburizers, Dissolution, Computer simulation, CFD Fluent

1. Introduction

During the gray cast iron melting one of the process stages is cast iron carburization. From among element occurring in cast iron carbon is most essential from microstructure point of view, which determine all mechanical, technological and utilitarian properties of castings. From carburizer quality and ability to make use of it depends liquid alloy quality, what influence on good casting quality and costs of it obtain. Good carburizers should to characterize with high carbon content in form of well-absorbing – graphite or carboids and low ash, sulfur, hydrogen and nitrogen content. On carburizer quality depends way of its dissolution in metal bath process.

1.1. Kinetics of carburization process

Carburization is a heterogeneous process, during which, according to W. Nernst, the following processes proceed:

- releasing of carbon from carburizer and formatting of boundary layer on carburizer surface,
- diffusional moving of carbon through the boundary layer adjacent to carburizer,
- carrying away of carbon deep to cast iron on the way of convectional-diffusional mass transport.

The biggest influence on dissolution rate in heterogeneous system have a speed of the slowest process, in this case it is second process that is diffusion of carbon through the boundary layer adjacent to carburizer (fig. 1.).

Accelerating of diffusion by the changing of temperature is insignificant, for the sake of limited abilities to change temperature of metallurgical processes.



Fig. 1. Carbon concentration in metal profile

Another factor, which has significant influence on dissolution rate, is a difference of reacting phase concentration. Carburization rate increases along with its rise.

By the set the movement to liquid phase, in which and between which takes place exchange of components, we can try to minimize diffusion distances. Along with speed of movement increase relative thickness of diffusional boundary layer clearly decrease. It is function of movement rate of liquid phase and its kinematic viscosity.

1.2. Simulation software CFD - Fluent

Software CFD (Computational Fluid Dynamics) make possible detailed analysis problems connected with fluid flow, eliminate necessity to carry out expensive and time-consuming experiments during cycle of devices design or modernization.

Software CFD also make possible to obtain indispensable information about flow of fluid (velocity distribution, pressure field), flow of heat (temperature field) mass transport (including chemical reactions). These are attained by numerical solution of equations describe momentum exchange, energy and mass balance. There are several numerical methods, which enable to solving mentioned equations, belong to them:

- finite element method,
- finite volumetric method.

Both first and second method owns advantages as well as some limitations dependent on class of analyzed matters. Fluent 6.2.16 system takes advantage of both methods so as to user has possibility to analyze as wide as possible group of matters [2].

1.3. Liquid metal movement in inductive furnaces

Very important matter enables to increase indexes of metallurgical processes is relative movement of inserting particles and liquid metal. It comes from decrease of, as a result of rotating movement of liquid metal, diffusion layer adjacent to carburizer particle. In inductive furnaces it is possible to control intensity of carburization process thanks to using furnaces with different power and frequencies.

Modern inductive average frequency furnaces have ability to change frequency for melting process and for inserting alloy additions for example from 400 to 200 Hz. Another solution is a power distribution on individual segment of furnace coil, it makes possible to force a movement in top layers of metal bath when the carburizer of alloy additions are inserted [3].

In dependence of coil current intensity, distance from furnace axis and depth of metal bath in these furnaces may be obtained velocity of liquid metal movement up to 3 m/s.

Much worse situation has place in electric arc furnaces, where intensity movement of metal bath take a place only near electrodes, however in the other space movement is slight or take place so-called "dead zone". In this case the best solution is pneumatic inserting to metal bath carburizer in stream of carrying gas. Transporting air fulfills two functions – delivers carburization material under the metal mirror and intensive mixing liquid metal [4, 5].

2. Calculation data

2.1. Geometry

Simplified two-dimension model of metal bath sector has been used in calculation (fig. 2.). Processes heating and dissolving of carburizer particle will be realized in 12x12x12 mm size cube filled with cast iron have been assumed. There is carburizer particle in the geometrical center of cube. On the basis of these assumption calculation of particle diameter depending on demanded carbon increase in liquid metal have been carried out.

Diameter of particle have been selected so as to mass fraction of inserted carbon amount to 3,1%. It comes from fact that in synthetic cast iron, melted on the basis of steel scrap, carbon deficiency, which have to be completed, amounts to 3,1%. In three-dimensions space this condition fulfils spherical 7 mm diameter particle.

As mentioned above simulations have been carried out on two-dimension model represents cube (12x12x12 mm) filled with cast iron about temperature 1723 K, initial temperature of particle amount to 300 K. Calculations for three carburizing materials: anthracite, graphite and petroleum coke have been carried out.



Fig. 2. Geometrical assumption

2.2. Relative movement rate of components

The relative movement of liquid metal and added carburizers has been supposed in the calculations. It comes from the fact that operation of carburization in induction furnaces or insertion of carburization in stream of compressed air has been assumed. Both in first and especially in second case intensive movement of metal bath occurs. Four levels of velocity have been supposed: 0 m/s, 0,01 m/s, 0,1 m/s and 0,5 m/s.

2.3. Thermophysical properties

Important issue in analysis of heat transfer process is knowledge about thermal conductivity coefficient (λ), specific heat (C_p) and thermal diffusivity (a). Dependence between these parameters is following: $\lambda = c_p \rho a$, where ρ is density.

Values of specific heat and thermal conductivity for graphite materials may be find in many publications [6, 7]. These data are similar to values from database of NovaFlow&Solid software, which are presented in table 3.

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Table 1.			
Thermophysical	properties	of grap	hite

T [°C]	0	200	600	1000	1600	2000
$\lambda [W/(mK)]$	135	103	79	47	21	12
c _p [J/(kgK)]	600	1170	1470	1930	2060	2170
a [mm ² /s]	118,4	46,33	28,28	12,82	5,37	2,91

Values of thermal conductivity for anthracite and petroleum cokes available in literature concern most often only temperature about 20°C and are significantly differ in value. Therefore the determination of specific heat and thermal diffusivity values was carried out, with laser impulse method on Netzsch 427 apparatus and scanning calorimeter Netzsch DSC 404C Pegasus, for anthracite, petroleum coke and synthetic graphite. Obtained values of thermal conductivity coefficient, specific heat and thermal diffusivity are presented in tables 2 and 3.

Table 2	Tal	ble	2
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Thermonhysical	properties of	netroleum coke
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T [°C]	16	499	1001	1499
λ [W/(m K)]	2,152	5,145	6,869	9,632
cp [J/(kg K)	780	1705	1970	2005
a [mm ² /s]	1,678	1,839	2,121	2,922

Table 3

Thermophysical properties of anthracite

T [°C]	16	499	999	1499
λ [W/(m K)]	1,663	3,011	3,299	3,875
cp [J/(kg K)	753	1635	1897	1913
a [mm ² /s]	1,319	1,100	1,039	1,210

The following densities have been supposed for these materials: for graphite -1900 kg/m^3 , for petroleum coke -1644 kg/m^3 and for anthracite 1674 kg/m^3 .

Following thermophysical properties of cast iron have been assumed, invariably in time function: λ =36 W/(m K), Cp=900 J/(kg K), ρ =7100 kg/m³.

3. Results

Example results of dissolution of anthracite particle simulation in form of carburizer concentration images in successive time moments as well as distribution of velocity vectors are presented in figures 3-9. In pictures 4-10 diagrams of change cast iron fraction along horizontal symmetry axis of model in time function for each relative movement rates are presented.

Influence of relative movement rate of components and kind of carburizer on course of changes maximum carburizer concentration in time function in analyzed domain is presented in figure 11.



Fig. 3. Dissolution of anthracite particle, in time t=0, t=0,05s and t=0,15s. Distribution of velocity vectors for v=0 m/s



Przekrój przez model [mm]

Fig. 4. Change cast iron fraction along horizontal symmetry axis of model in time function for v=0 m/s



Fig. 5. Dissolution of anthracite particle, in time t=0, t=0,05s and t=0,15s. Distribution of velocity vectors for v=0,01 m/s



Przekrój przez model [mm]

Fig. 6. Change cast iron fraction along horizontal symmetry axis of model in time function for v=0,01 m/s



Fig. 7. Dissolution of anthracite particle, in time t=0, t=0,02s and t=0,05s. Distribution of velocity vectors for v=0,1 m/s



Przekrój przez model [mm]

Fig. 8. Change cast iron fraction along horizontal symmetry axis of model in time function for v=0,1 m/s



Fig. 9. Dissolution of anthracite particle, in time t=0, t=0,005s and t=0,025s. Distribution of velocity vectors for v=0,5 m/s



Przekrój przez model [mm]

Fig. 10. Change cast iron fraction along horizontal symmetry axis of model in time function for v=0,5 m/s



Fig. 11. Maximum carburizer concentration in analyzed domain

4. Conclusions

On the basis of carried out simulations of carburizing materials in liquid metal dissolution process, one may comes to following conclusions:

- Graphite particle, i.e. highest density material, dissolves slowest it is especially noticeable in minimal relative movement rate conditions. But taking into account heating process [11], which is proceeds fastest for graphite, one can affirm that carburization process will be shortest for graphite next for petroleum coke and next for anthracite.

- Relative movement of carburizer particle and metal bath wit speeds 0,1 i 0,5 m/s significantly accelerate process of carburizer dissolution and what follows carburization process. Influene of kind of carburization material on this realation is insignificant.

- One of the ways to further intensification of dissolution process is enlargement reaction surface between carburizer and metal bath by reduction particles size with, in the same time, increasing they amount. In the heating case it is more significant than relative movement rate [11] one should to suppose that in dissolution case will be similarly.

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