BEHAVIOR OF Y_2O_3 AND Al_2O_3 PARTICLES NEAR THE SOLIDIFICATION FRONT

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Abstract

The performed tests were focused on the mechanism of reaction of Y_2O_3 and Al_2O_3 particles with the solidification front while casting steel. The presence of oxide inclusions in steel is a consequence of precipitation and segregation processes in the CCM crystallizer. The oxide precipitations in the liquid metal are a result of deoxidization and are generally unfavorable for the future properties of steel; on the other hand, their fine dispersive phase may play the role of nucleation centers of other phases, which in this case is advantageous. Yttrium oxide precipitations are formed when yttrium is used as a modifier and micro additive to steel of definite properties. Unlike Al_2O_3, the resulting Y_2O_3 phase may be advantageous because it strengthens steel. Considerable differences between the density of aluminum oxide and yttrium oxide affect their interaction with the crystallization front. This will decide about the final distribution of inclusions in the cast ingot. Authors suggested a numerical solution with the use of own computer program. During computations a system of forces that acts on particle as well as physicochemical parameters of steel were taken into account. The calculations were performed in micro scale in reference only to one particle of a given radius, occupying different position with respect to the solidification front. The results of calculation were presented in the form of plots illustrating the change of position of the particle of a given radius with respect to its initial position.

Keywords: Solidification front, Y_2O_3, Al_2O_3, numerical modelling, precipitation movement

1. INTRODUCTION

The simplest criterion, in which free energy of absorption ΔG_p is defined, should be used for checking out whether or not a solidification front absorbs particles. It is expressed as a difference of interface energy (inclusion/solid metal) and (inclusion/liquid metal). The absorption takes place when the following condition holds true:

$$\Delta G_p = \sigma_{i-s} - \sigma_{i-l} \leq 0, \tag{1}$$

where: $\sigma_{i\text{-}s}$ - surface energy of inclusion/solid metal (N / m), $\sigma_{i\text{-}l}$ - surface energy of inclusion/liquid metal (N / m), ΔG_p - free energy of absorption.

The flat crystallization front moves vertically at a constant velocity V_{st}. The behavior of the particle is a result of balance of forces acting on it. Gravity force [1-4,8]:

$$F_g = \frac{4}{3}\pi r^3 (\rho_m - \rho_i) g, \tag{2}$$

where: F_g - gravity force (N), ρ_m - density of metal (kg / m^3), ρ_i - density of inclusion (kg / m^3), g - acceleration of particles (m / s^2), r - radius of inclusion (m).

The viscous resistance force, which is opposite to the direction of the particle moving at velocity V_i with respect to fluid, is presented in the following form[1,5-8]:

$$F_d = 6\pi \mu r V_i \theta, \tag{3}$$

where: F_d - viscous resistance force (N), μ - coefficient of dynamic viscosity (kg / (m·s)), V_i - flow rate of inclusion with respect to fluid (m / s),

The value of coefficient θ depends on the distance from the front h and direction of particle movement:

for inclusion distant from the front θ = 1, - for inclusion approaching the front θ = r / h, for inclusion moving parallel to the front θ = ln(r / h).

The unevenness of concentration of components making up the liquid and different velocities are a frequent phenomenon. The force generated by the gradient of fluid velocity S, acting perpendicular to the front surface, in the area which can be defined as a boundary layer of velocity, is called Saffman force and is expressed by the formula [1-8]:

$$F_s = 6.46\,\mu\, r^2 V_i \sqrt{\frac{S}{v}} \tag{4}$$

where: F_s - Saffman force (N), v - kinematic viscosity (m^2 / s), S - local gradient of fluid rate (s^{-1}).

Such force may cause moving away or approaching of a particle to the front, depending on the direction of the fluid and difference of density of particle and fluid. Saffman force makes the particle move away from the front, when the fluid flows down the front, and when the density of the particle is bigger than that of the fluid.

Presented work focuses on numerical modelling of Y_2O_3 and Al_2O_3 precipitants behaviour near to the solidification front while casting steel. The mathematical model of solidification front influence on the particle movement base on the balance of forces that acts on it. Numerical solution of this model allows to understand the behavior differences of yttrium and aluminium oxides in liquid steel during solidification.

2. NUMERICAL MODEL FOR A PARTICLE MOVING CLOSE TO THE SOLIDIFICATION FRONT

Particle movement near the crystallization front may be described with the following mathematical model [8]:

$$a = \frac{\left|F_w\left(F_S, F_g, F_d, v\right)\right|}{\frac{4}{3}\pi\, r^3 \rho_{cz}}$$

$$\begin{cases} \dfrac{dv_x}{dt} = a_x, \\ v_x(t=0) = v_x^0 \end{cases} \tag{5}$$

$$\begin{cases} \dfrac{dv_y}{dt} = a_y, \\ v_y(t=0) = v_y^0 \end{cases}$$

where: a - vector of particle acceleration, a_x - acceleration vector component in x axis direction, a_y - acceleration vector component in y axis direction, v - vector of particle speed, v_x - speed vector component in x axis direction, v_y -speed vector component in y axis direction, v_x^0, v_y^0 - initial values of speed, taking into account fluid gradient, r - substitute particle radius, ρ_{cz} - particle density, F_w - resultant force vector, F_S - Saffman force vector, F_g -buoyancy force vector, F_d - liquid resistance force. Result of the modeling is location of the particle at each and every moment in time: ($x(t)$, $y(t)$), which can be described with following set of ordinary differential equations:

$$\begin{cases} \dfrac{dx}{dt} = v_x, \\ x(t=0) = x^0 \end{cases} \qquad \begin{cases} \dfrac{dy}{dt} = v_y, \\ y(t=0) = y^0 \end{cases} \tag{6}$$

To define force components that act on the particle in x and y direction directional trigonometric functions of resultant force F_w were taken into account.

Liquid in the analyzed domain can flow relatively close to the crystallization front. Its flowing speed can be described in *x* and *y* separately. Those values affect the particle movement. At the stage of numerical solving the liquid movement speed components are added to initial values of particle speed components. To solve a set of ordinary differential equations presented above (eqs. 2, 3) Euler's forward scheme with constant time step Δt is applied. The aim of the computations is to create the numerical sequence of the following values:

$$\left(t^n, x^n, y^n, v_x^n, v_y^n\right), \quad n = 1, 2, 3, \ldots \tag{7}$$

which values are approximate positions and particle speeds at equidistant time steps.

After each and every time step the acceleration a value is updated as its value depends on the resultant force vector (eq. 1). Based on the numerical model given above computational procedures were prepared and the original software was written.

3. RESULTS OF CALCULATION AND DISCUSSION

The simulation was performed with the use of a computer program, based on the equation of forces acting on a particle and also mathematical and numerical model. The following parameters were assumed for steel and the particle (**Table 1**) [9, 10]:

Table 1 Material data and calculation parameters

steel density	7874 kg / m^2
particle density	Y_2O_3 - 5010 kg /m^3; Al_2O_3 - 3990 kg / m^3
dynamic viscosity	0.06 m^2 / s
time step	$1 \cdot 10^{-6}$ s
local velocity gradient	0.0001; 0.00001; 0.000001 s^{-1}
particle radius	10, 20, 50 μm

Calculations were performed for a particle at a considerable distance from the front and for a particle approaching the front. The interaction was analyzed for particles of radius 10, 20 and 50 μm and local velocity gradient 0.0001; 0.00001; 0.000001 s^{-1}. In each case the calculation time was the same, i.e. 10 s. The first calculation series was performed for particles staying at a distance from the solidification front (**Figures 1 - 3**). It was assumed that the velocity gradient had an influence on the trajectory of the particle therefore it was not accounted for in the calculations. The interaction with the front was observed to be the biggest for a big gradient of velocity; the particle moved towards it. The interaction of particles with the front are negligibly small for low and moderate gradients. The same dependence can be observed for each particle size.

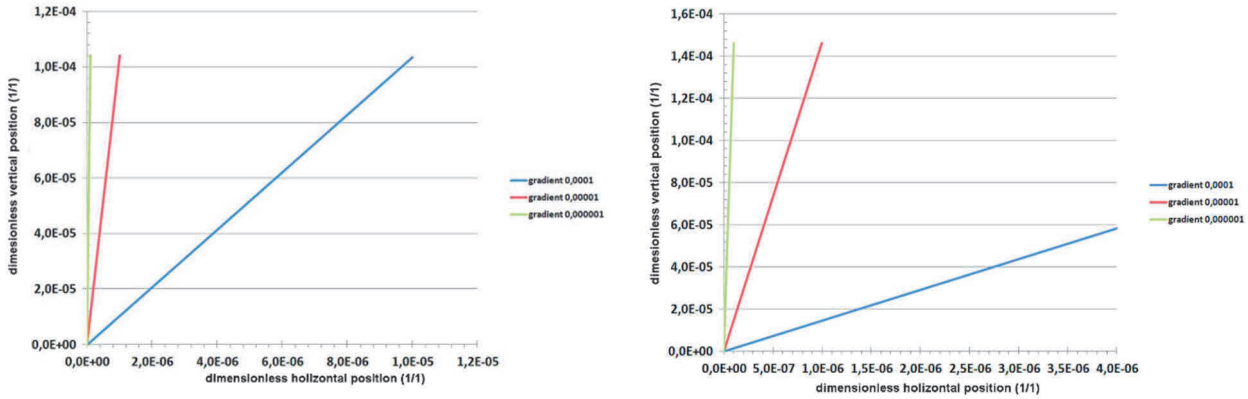

Figure 1 Influence of local gradient on the movement of particle of radius 10 μm: left plot - Y_2O_3 particle; right plot - Al_2O_3 particle

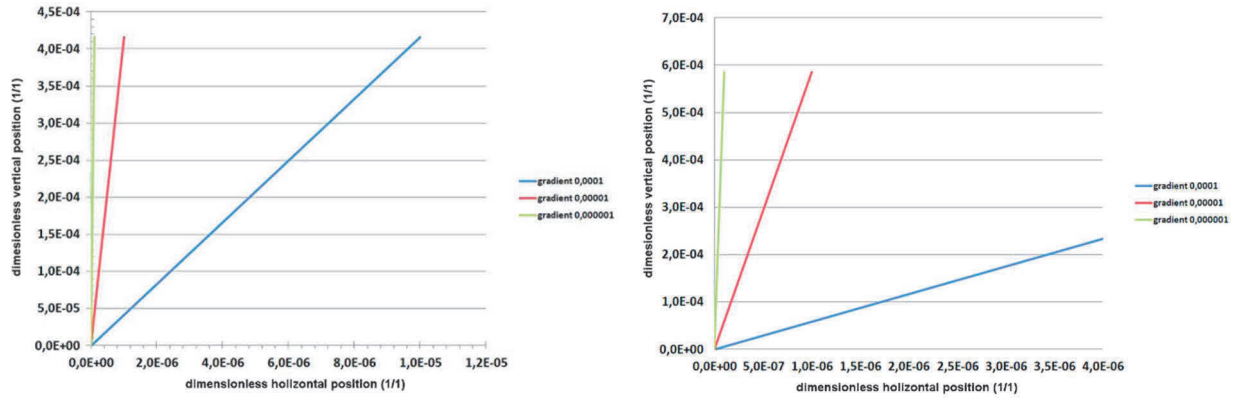

Figure 2 Influence of local gradient on the movement of particle of radius 20 μm: left plot - Y_2O_3 particle; right plot - Al_2O_3 particle

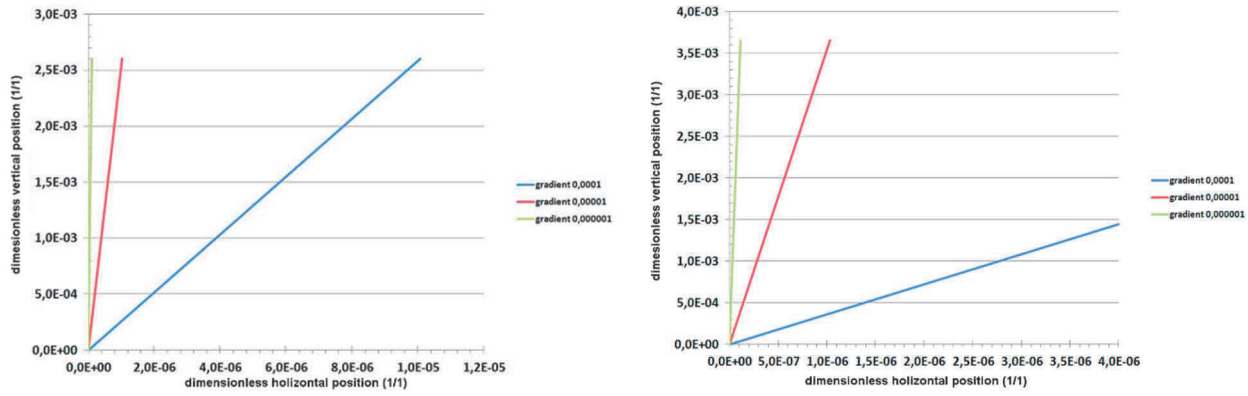

Figure 3 Influence of local gradient on the movement of particle of radius 50 μm: left plot - Y_2O_3 particle; right plot - Al_2O_3 particle

An analogous simulation was conducted for a particle approaching the front. The results of calculations for particles of radius 10, 20 and 50 μm are presented in **Figures 4 - 7**.

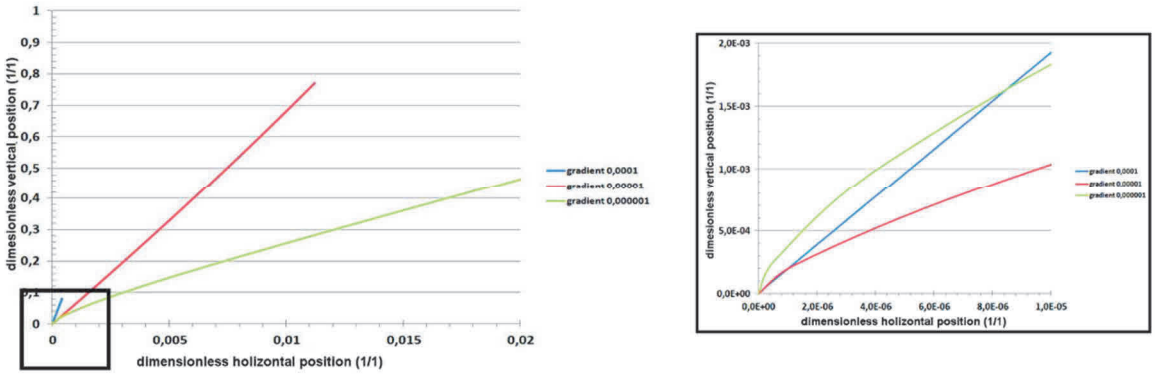

Figure 4 Influence of local gradient on the movement of Y_2O_3 particle of radius 10 μm

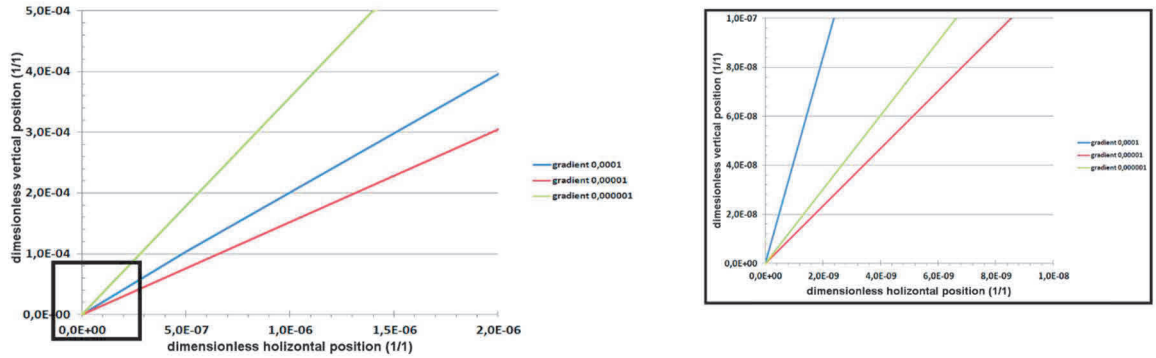

Figure 5 Influence of local gradient on the movement of Al_2O_3 particle of radius 10 μm

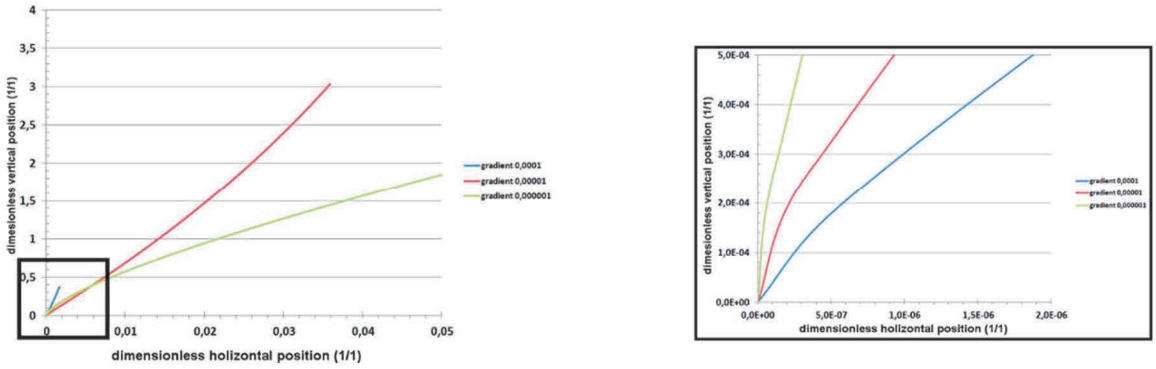

Figure 6 Influence of local gradient on the movement of Y_2O_3 particle of radius 50 μm

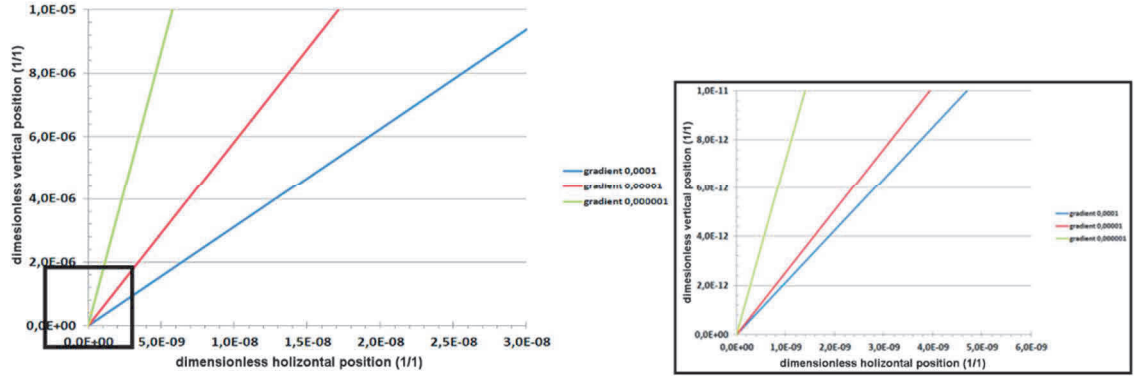

Figure 7 Influence of local gradient on the movement of Al_2O_3 particle of radius 50 μm

Additional plots were presented to illustrate the behavior of a particle at the initial phase of the beginning stage. The case of a particle approaching the front at a given gradient of velocity clearly shows the effect of its operation on the particle trajectory. In all analyzed cases the behavior of low velocity gradient makes the particle move towards the front and flow out on the surface.

4. CONCLUSION

Local gradient of velocity of liquid phase is important for the movement of the particle regardless the size of the inclusion, at the assumed location of the particle at a distance from the crystallization front, also for particles moving towards the front. In the first case, at a small gradient of velocity the particle freely flows out to the surface of liquid metal, due to the operation of the buoyancy force Stokes mechanism. Here the interaction of the inclusion and the front are negligible. Only after obtaining a definite value of gradient of velocity of liquid metal 0.001 s^{-1} causes that the particle trajectory is oriented towards the solidification front. This trend was observed for all analyzed particle sizes, i.e. 10, 20 and 50 μm. In analogous simulations made for a particle moving towards the front the particle trajectory was observed to significantly deflect towards the front for the lowest gradient of velocity of liquid metal. This tendency was maintained for all radiuses of the analyzed particles.

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