Mathematical modeling of the process of carbon bubbles formation in the interaction of a gas jet and a melt bath in the oxygen converter

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Abstract. The article discusses the issues of modeling the processes of interaction of gas jets and metal melt during blowing of a converter bath. The authors developed and implemented using the finite element method a mathematical model based on a direct numerical solution of the Navier-Stokes equation without using a turbulence model. This model helped to study the dynamics of the velocity field and the boundary of the penetration of the jet into the metal. According to the results of mathematical modeling, a mechanism for the formation of carbon monoxide bubbles is suggested.

1. Introduction

In the top-blown converter, a jet of oxygen at a supersonic speed is directed by means of a lance to the bath of molten metal. In this case, two processes are realized: the formation of a cavity on the surface of the bath due to the dynamic pressure of the jet and the formation of a vortex flow in the volume of whole bath. The size, shape and boundary of the cavity are important parameters that determine the decarburization of cast iron in the bath, accompanied by the formation of carbon monoxide, which can react with oxygen in the upper space of the converter to form carbon dioxide.

This latter process is usually called the afterburning reaction, the exothermic effect of which is at twice the decarburization reaction [1]. Therefore, the creation of optimal conditions for the afterburning of carbon monoxide in the cavity of the converter is an actual scientific and practical task [2].

Experimental studies on the problem of a gas jet collision with a liquid surface, starting from [3] in the 60’s to later experiments [4 –6], were carried out using reduced cold models in which oxygen was replaced by air and molten steel was replaced by water. In these experiments, the integral dimensions and surface shape were investigated, while the local deformation of the cavity boundary was not considered.

The modeling of deformations of the free bath surface and the flow in a metal under the influence of jets was considered in numerous works, for example, in [7–12]. In [8], a physical and mathematical model of the instability in the behavior of the bath boundary was proposed. Model [9] describes the fluctuations of the melt level. In [10], a numerical study of the interaction between jets and a slag-metal bath is presented using a three-phase volumetric model of a liquid. Numerical results show that the cavity profile and the slag/metal/gas interface remain unstable as a result of the propagation of surface waves, which is probably the main factor determining the generation of metal droplets and
their initial spatiotemporal distribution. Recent reviews [11, 12] present data on the interaction of an oxygen jet with a molten bath based on the volume of fluid method (VOF) using one or another turbulence model. Turbulence models use turbulent viscosity, which significantly exceeds molecular viscosity, which allows calculating mixing processes over a long period of time in the melt pool and in the upper space of the converter. However, this leads to a loss of flow detail. If to refuse the use of turbulent viscosity, important details of the process can be noted, for example, the formation of bubbles at times of one tenth of a second.

The works on the phenomena occurring in the upper space of the converter and on afterburning are mainly empirical in nature [13], where it was found that the afterburning coefficient in the exhaust gases, defined as the ratio of the concentration of carbon dioxide to the total concentrations of CO and CO₂, increases with the increase in height of the lance. An increase in the temperature and carbon content in the bath leads to lower values of this indicator.

2. Problem statement and solution method

Let us consider the interaction of a gas jet of the converter moving with speed \( u_0 \) and a bath of melt with the physical characteristics presented in table 1.

The motion of gas and melt is described by the Navier-Stokes equation for a viscous incompressible medium:

\[
\frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{F}_g
\]

\( \nabla \cdot \mathbf{u} = 0 \) \quad (1)

Where \( \mathbf{u} \) is the velocity vector, \( p \) – pressure, \( \mathbf{F}_g \) – volumetric gravity, \( \rho \) – density, \( \mu \) – dynamic viscosity.

This system was solved numerically in a flat coordinate system using the finite element method. The finite element mesh is shown in figure 1. A conservative Level Set method was used to track the interface between the melt and gas. The method consists in calculating the scalar function for the entire computational domain:

\[
\rho \left( \frac{\partial \phi}{\partial t} + \nabla (\phi \mathbf{u}) \right) = \chi \left[ \varepsilon \nabla \cdot \nabla \phi - \nabla \cdot \left( \phi (1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \right] \quad (2)
\]

Where \( \varepsilon \) is the parameter determining the thickness of the transition layer and equal to half the size of the mesh cell, \( \chi \) is the stabilizing parameter equal to the maximum speed achieved in the calculation area. In the transition zone, the density, viscosity, and electrical conductivity are approximated:

\[
\rho = \rho_s + (\rho_n - \rho_s) \phi, \\
\mu = \mu_s + (\mu_n - \mu_s) \phi
\] \quad (3)

The surface tension force is calculated by the formula:

\[
\mathbf{F}_s = \nabla \cdot \left[ \left( \frac{\gamma (\mathbf{I} - \mathbf{n} \mathbf{n}^T)}{\nabla \phi} \right) \delta \right], \\
\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}, \quad \gamma = \phi (1-\phi) |\nabla \phi| \quad (4)
\]

Where \( \mathbf{I} \) is the identity matrix, \( \mathbf{n} \) – the normal vector to the surface, \( \gamma \) – the surface tension coefficient, \( \delta \) – the Dirac delta function, which is not equal to zero only on the contact surface.
Table 1. Geometric and physical characteristics.

| Designation | Value  | Description               |
|-------------|--------|---------------------------|
| $H$         | 5.254 m| Estimated converter height|
| $H_w$       | 2.27 m | Melt layer height         |
| $D$         | 7.42 m | Converter diameter        |
| $U_0$       | 500 m/s| Gas velocity              |
| $\rho_g$   | 0.23 kg/m$^3$ | Gas density              |
| $\mu_g$    | $0.73 \cdot 10^3$ Pa·s | Dynamic gas viscosity |
| $\rho_m$   | 8136 kg/m$^3$ | Melt density             |
| $\mu_m$    | 0.0058 Pa·s | Dynamic melt viscosity   |
| $D_{out}$  | 50 mm  | Lance nozzle diameter     |
| $T_0$      | 1812 K | Initial temperature       |
| $\sigma$   | 1 N/m  | Surface tension coefficient|

Figure 1. The calculated finite element mesh.

2.1. Initial and boundary conditions

At the initial moment of time, the melt is at rest, and the gas flows at a speed $u_0$. On the walls of the tuyere the adhesion condition is set:

$$ u = 0 $$  \hspace{1cm} (5)

Figure 2 presents the results of calculations of the velocity field of jet penetration into the metal for various time instants, from which the instability of the interface follows. The development of instability leads to the formation of metal droplets (Figure 2 a-c) and the gas bubble inside the liquid (figure 2 c). This suggests a mechanism for the formation of carbon monoxide bubbles. The bubble formed due to instability, the oxygen of which interacts with carbon (a heterogeneous reaction), turns into carbon monoxide. Under the influence of Archimedean forces, this bubble rises to the surface and bursts. Then the upward hydrodynamic flow carries carbon monoxide into the upper space of the converter.
Figure 2. Speed fields during the jet penetration into the metal.
3. Conclusion
The direct method of numerical simulation of the Navier-Stokes equations solved the problem of the interaction of a supersonic gas jet with a liquid metal. The distributions of the velocity field and the geometry of the gas-liquid interface for various time instants are obtained. The obtained interface form proves that hydrodynamic instabilities are realized on it, leading to the formation of metal particles in the gas and gas bubbles in the metal. The analysis of the hydrodynamic situation made it possible to propose a mechanism for the formation of carbon oxide bubbles.

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