Mathematical modelling of the liquid atomization process by cocurrent gas flow

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Abstract. This paper focuses on the physical-mathematical model of liquid atomization in the spray pattern of an ejection nozzle. A flow field of a gas phase behind the nozzle section is computed using the Ansys Fluent package. Dynamics of molten metal droplets in the gas phase within a trajectory approach is calculated. Using the presented model, numerical calculation results are given.

1. Introduction
In metallurgy, spraying techniques involving ejection nozzles are widely used to produce the high-dispersive powders from molten aluminum \cite{1-3}. The jet of molten aluminum is dispersed by a hot nitrogen flow. It results in formation of poly-dispersed droplets that are crystallized in the form of powder of a termination product in cases of refrigeration in a sedimentation chamber. The morphology of the aluminum particles is significantly affected by time and dynamics of a phase change of the particles.

This study includes the results of mathematical modeling for a two-phase flow in the spray pattern of an ejection nozzle.

2. Results and discussion
2.1. Calculation of a flow field of a gas phase
The problem of gas jet efflux in a sedimentation chamber is considered in a non-viscous formulation using Eulerian equation in a perfect gas \cite{4}. It is assumed that the flow is axisymmetric. Figure 1 shows the scheme of the computational region. The hot gas (nitrogen) is supplied through channel 1 through section AB. In the tapered section of the channel it is accelerated to a sonic velocity that is achieved in the vicinity of cross section CD. Then the hot gas moves in sedimentation chamber 2. In the working chamber the gas velocity in the jet initially increases up to a supersonic one and then it gradually decreases moving from the nozzle.
The flow field is described by Eulerian equations:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{1}{r} \frac{\partial}{\partial r} (\rho vr) = 0, \\
\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2) + \frac{1}{r} \frac{\partial}{\partial r} (\rho uv) = -\frac{\partial p}{\partial x}, \\
\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (\rho uv) + \frac{1}{r} \frac{\partial}{\partial r} (\rho vr^2) - \frac{\rho u^2}{r} = -\frac{\partial p}{\partial r}, \\
\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x} [\mu(\rho E + p)] + \frac{1}{r} \frac{\partial}{\partial r} [\nu(\rho E + p)r] = 0.
\]

Here \( x, r \) are the axial and radial coordinates; \( t \) is the time; \( \rho \) is the density; \( u, v \) are the axial and radial components of the velocity; \( p \) is the pressure; \( E = h - \frac{p}{\rho} + \frac{1}{2}(u^2 + v^2) \) is the total energy per unit mass; \( h = C_p T \) is the static specific enthalpy; \( C_p \) is the specific isobaric heat capacity; \( T \) is the temperature.

The system of Eulerian equations is supplemented by the equation of state:

\[ h = \frac{\gamma}{\gamma - 1} \frac{p}{\rho}, \]

where \( \gamma \) is the adiabatic index.

Eulerian equations are solved with the following boundary conditions.

In cross section AB the values of the stagnation temperature, Mach number and gas pressure were predetermined; on the boundary of regions GH and FH the values of undisturbed pressure were predetermined, \( p = 10^5 \) Pa; on walls CE, DG the impermeability condition was imposed. The problem was solved using program package ANSYS Fluent 13.0.

A computational grid was composed of about 44000 meshes. Across the channel, 20 meshes were taken; in the working chamber the grid with the size of a mesh less than 1 mm was nonregular.

The problem was solved by explicit Rau method with the first order of both time and spatial variable approximation. Quiescent conditions with undisturbed pressure and temperature values were assigned as an initial field. The Courant number in the calculations performed was equal to 0.8. During solution of the problem, the flow field appearing in cases of ingress of the jet from the initial cross in the channel firstly and then in the working chamber was determined. The calculation was conducted up to physical time \( t = 10^{-4} \) s. The calculation time was equal to about 4 hours using PC with CPU frequency of 2 GHz. In this interval of time, the establishment of the flow field was not
completely achieved but the picture in the vicinity of the nozzle changed. Figures 2, 3 show the typical results of the numerical calculation.

**Figure 2.** Mach number in the working region.

**Figure 3.** Pressure field in the working chamber.

During the calculations, the geometrical sizes of the region were assigned using the conditions of technical requirements. At the channel input (the cross section AB) the values of stagnation temperature $T = 773$ K, pressure $p = 6.08 \times 10^6$ Pa and Mach number $M = 0.055$ were assigned.

Figure 2 shows the distribution of Mach number in the working chamber. In the working chamber the jet comes with a nonuniform velocity profile. Mach number averaged over the cross section is equal to about 1.5. Then in the vicinity of the nozzle the jet is accelerated up to $M \approx 5$ due to nozzle divergence. The velocity decreases along with the increase of the distance from the nozzle. In the vicinity of the symmetry axis the flow always remains subsonic. Figure 2 clearly shows the contours of the jet.

Figure 3 shows the structural contours of the pressure field in the sedimentation chamber. At the outlet from the nozzle in cross section CD the pressure is nonuniform; it changes from $10^6$ Pa on the lower edge of the cross section (near point C) to $2.9 \times 10^6$ Pa on the upper edge of the cross section (point D). In the sedimentation chamber in the jet core the pressure falls up to $0.96 \times 10^4$ Pa, while moving from the jet the pressure increases.

During the quantitative estimation of parameters of the hardening process it is necessary to take into account the change of the particles velocity. The particles that are involved in motion by a gas flow due to drag forces with time tend to equalize their velocity with the velocity of the gas flow. It results in a sufficient decrease in their heat exchange with carrying medium. Both the cooling time of particles (depending on a particles size) and the time of the hardening process essentially grow. As a result, the parametric analysis of the cooling process of the molten metal particles and their hardening taking into account the change of the particle motion velocity at constant values of the gas velocity and temperature has been conducted.
2.2. Calculation of a motion path of a particle

An equation for movement of particles with constant radius \( r \) at constant velocity \( u \) and density of the blowing gas \( \rho \) is as follows:

\[
\frac{4}{3} \pi^2 \rho \frac{d\nu}{dt} = \pi r^2 C_D \frac{\rho(u - \nu)|u - \nu|}{2},
\]

where \( \rho_p \) is the density of the particles.

The drag coefficient was determined by Klyachko-Mazin’s formula:

\[
C_D = \begin{cases} 
\frac{24}{Re} + \frac{4}{\sqrt{Re}} & Re < 900; \\
0.44 & Re \geq 900,
\end{cases}
\]

where \( Re = \frac{2\rho_p|u - \nu|}{\mu} \) is the Reynolds number; \( \mu \) is the factor of the dynamic viscosity of the streaming gas.

We integrated equation (1) for the corresponding Reynolds numbers taking into account (2) and obtained dependence \( Re(t) \) for the whole period of the particle motion

\[
Re(t) = \begin{cases} 
\frac{6\sqrt{6}}{6}, & Re(t) < 900; \\
\frac{\mu}{1 + 0.165 \frac{\rho}{\rho_p}|u - \nu_0|t}, & Re(t) > 900.
\end{cases}
\]

The comparison of the calculation results on analytical dependence of equation solution (1) and numerical solution showed that they practically coincide at integration step \( \Delta t = 10^{-7} \).

Figure 4 shows the typical calculation results for different particles sizes.

![Figure 4](image)

**Figure 4.** Dependence of the particle movement velocity on time; gas velocity is 800 m/s.

The analysis of the aluminum particles movement taking into account the flow parameters of carrying medium was conducted for specified conditions of the sedimentation chamber. Figure 5 shows the motion pattern that is obtained for the known flow field (without considering the inverse impact of particles on the gas medium) within the trajectory approach. Coordinate of the point of the particles injection in the cross section \( x = 0 \) is radius \( r = 8 \) mm that is measured from the axis of the atomizing nozzle.
The evolution of the particle motion pattern is determined by a significant value of the radial velocity of the gas that is directed to the axis of the nozzle due to free jet expansion. Then, the particles movement is determined by the parameters of the jet along with the increase of the distance from the injector exit (Figures 2, 3).

![Figure 5. Trajectories of the particles movement in the sedimentation chamber in the vicinity of the nozzle.](image)

2.3. Experimental study
The experimental study was carried out to verify the calculation results using the Particle Image Velocimetry method (PIV-method). PIV-method is a widely accepted method for measuring of the velocity field of particles in a fluid and gas flow [5]. Figure 6 shows the structure of the gas jet at different values of the pressures ratio in the supply chamber and ambient medium $N_{pr}$.

![Figure 6. PIV-diagnostics of the velocity field of jet and stream lines of gas: $a - N_{pr} = 2$; $b - N_{pr} = 5$; $c - N_{pr} = 9$.](image)
Figure 7 shows a photograph of a gas jet at value $N_{pr} = 9$.

![Figure 7. Visualization in a laser knife.](image)

### 3. Conclusion

The analysis of the numerical results using two approaches to a mathematical description of the crystallization process of the aluminum particles in a spray pattern of the injection nozzle has showed:

– the rate of throughput and stagnation temperature of atomizing gas in the ranges, which are used in the industrial aluminum powder ASD technology, practically does not influence the characteristics of crystallization;

– approximation dependences of the characteristics of the crystallization process (duration of the crystallization process, moment of the time and coordinate along the axis of the jet that corresponds to the beginning of the crystallization, length of the crystallization region) on aluminum particles sizes.

The presented results allow optimizing technological parameters of injection nozzles for obtaining the particles of powder with the specified morphology.

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