Analysis the dynamics formation of a vapor supersonic jet under outflow from thin nozzle

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Abstract. The dynamics formation of a vapor jet with near-critical state parameters outflowing from a high-pressure vessel through a thin nozzle is studied. The numerical modeling of this process, by using a system of model equations for gas-vapor-liquid mixture, which include conservation laws of mass, momentum, and energy of phases in accordance with one-pressure, one-velocity and two-temperature approximations, was conducted, taking into account heat and mass transfer processes of evaporation and condensation under conditions of equilibrium state with modified reacting TwoPhaseEulerFoam solver of open package OpenFOAM. The process of barrel shock formation in supersonic boiling jet with shaping Mach disk is shown. It was found that the process of boiling fluid outflow is accompanied by formation of vortex zones near axis of symmetry and leads to generation of acoustic wave pulses series preceding the main jet flow, which are the source of pulsations, observed in experiments. The justification of applied numerical method reliability is shown by comparing the computational and analytical solutions for Sedov’s problem of a point explosion in gas-water mixture at the plane case.

1. Introduction
Recently, interest in study of a vapor jet streams formation is associated with their wide application in various technologies for spraying liquids and with problems emergent from sudden depressurization of high-pressure vessels under critical state parameters. Analysis the dynamics of such jets is necessary when solving safety problems of modern power equipment in order to prevent accidents.

In the work [1] were studied the processes of gas jets evolution, accompanied by formation of Mach disks and occurrence of vortex rings. In [2], [3] experiments were conducted out to study the outflow of superheated water from a high-pressure vessel through a short cylindrical nozzles. The angle of jet disintegration, depending on various regimes factors and initial conditions, was determined.

In [4], [5] the process of water outflow from initial supercritical pressure at the end rupture of pipeline was investigated numerically. The influence of initial water state in a high-pressure vessel, taking into account the intensity of boiling water nucleation, on evolution of the steam-water jet shape at incipient stage of outflow under experimental conditions [2], is analyzed in the work [6] using the Lagrangian approach.

For further studies of vapor outflow problem, initially located at high pressure in a supercritical state [7], the solver of OpenFOAM package was used. The calculations were carried
out for longer times to subsequent stages of jet formation which were performed in a single-phase approximation, when it is possible to ignore evaporation and condensation processes.

This work is a continuation of studies considered problem [7] in accordance with the experimental conditions close to [2], [3], and taking into account the model representations describing a gas-vapor-liquid mixture with heat and mass transfer processes. The numerical implementation of model equations was carried out using the modified by authors reactingTwoPhaseEulerFoam solver from the OpenFOAM package.

2. Problem statement and model equations

To study the dynamics of a high-temperature jet formation the following problem was solved. At the initial moment of time, a water fluid was located in a cylindrical pressure vessel of depth \( x_h = 10 \) mm and radius of \( y_h = 10 \) mm under pressure \( p_0 = 9.45 \) MPa and temperature \( T_0 = 600 \) K [2]. After the diaphragm rupture through a narrow cylindrical nozzle with a radius of \( y_s = 0.25 \) mm and a length of \( x_s = 0.5 \) mm, the outflow of superheated vapor into undisturbed surrounding air environment, staying at \( p = 0.1 \) MPa, \( T = 300 \) K, occurred. The computational domain scheme corresponding to experiment [2] is shown on Fig. 1 on the left fragment. In the right part of the same figure is shown the photograph of boiling fluid jet [2], corresponding to the regime of homogeneous boiling that occurs in terms, which comparable to the above mentioned conditions of outflow with a jet shape, close to parabolic.

To model and numerically study considered process the system of model equations for two-phase gas-vapor-liquid mixture [8]-[10] was used, which includes the conservation laws of mass, momentum, and energy of each phase in accordance with one-pressure, one-velocity, and two-temperature approximations, taking into account heat and mass transfer processes of evaporation and condensation. Below are the basic model equations:

continuity equations of phases:

\[
\frac{\partial (\alpha_i \rho_i)}{\partial t} + \text{div} (\alpha_i \rho_i \vec{v}) = \Gamma_i, \tag{1}
\]

momentum conservation equations of phases:

\[
\frac{\partial (\alpha_i \rho_i \vec{v})}{\partial t} + \text{div} (\alpha_i \rho_i \vec{v} \vec{v}) = -\alpha_i \nabla p + \text{div} (\alpha_i \vec{\tau}_i) + \Gamma_i \vec{v}, \tag{2}
\]

where \( \vec{\tau}_i = \mu_i (\nabla \vec{v} + \nabla \vec{v}^T) - \frac{2}{3} (\mu_i \text{div} \vec{v}) I \) – viscous stress tensor of \( i \) – phase;

energy conservation equations of phases:

\[
\frac{\partial (\alpha_i \rho_i (e_i + K_i))}{\partial t} + \text{div} (\alpha_i \rho_i \vec{v} (e_i + K_i)) = -p \frac{\partial \alpha_i}{\partial t} - \nabla (\alpha_i \vec{v} p) + \text{div} (\alpha_i \vec{v} \cdot \vec{\tau}_i) + \text{div} (\alpha_i \gamma_{i,\text{eff}} \nabla h_i) + K_{hi} \Delta T + L_i \Gamma_i, \quad \gamma_{i,\text{eff}} = \frac{c_{p,i}}{c_{V,i}} \gamma_i. \tag{3}
\]

The mass transfer rate \( \Gamma_i = \frac{\partial m_i}{\partial t} \) is determined by the intensity of evaporation (condensation) process in the equilibrium saturation state described by Antoine’s equation [10].

In equations (1)–(3) the following notations were used: \( \vec{v} \) – mass velocity vector, \( p \) – pressure, \( \rho_i \) – density, \( \alpha_i \) – volume fraction content, \( c_{p,i} \), \( c_{V,i} \) – specific heat capacities at constant pressure and volume, \( \gamma_i \) – thermal diffusivity, \( \gamma_{i,\text{eff}} \) – effective thermal diffusivity, \( e_i \) – internal energy, \( K_i \) – kinetic energy, \( h_i \) – enthalpy, \( T_i \) – temperature, \( L_i \) – latent heat of vaporization/condensation, \( K_{hi} \) – heat transfer coefficient, \( I \) – unit tensor. The subscript \( i = 1, 2 \) corresponds to liquid and vapor phases. The thermodynamic properties of water and vapor are described by perfect equations of state.
Figure 1. On the left: scheme of the computational domain: 1 – high-pressure vessel, 2 – nozzle, 3 – jet formation zone, 4 – symmetry axis. On the right: photograph of boiling fluid jet [2].

3. Numerical simulation method and accuracy verification

The computer implementation of proposed model for gas-vapor-liquid mixture was carried out using a modified by the authors reactingTwoPhaseEulerFoam solver of OpenFOAM package. It was built on the basis of PIMPLE computational algorithm, which significantly accelerates calculations and allows to achieve a good convergence rate of solutions. The integration of partial differential equations for each control volume ensures the conservatism of numerical scheme.

To assess the reliability of proposed numerical simulation method, the comparative analysis of computing realization using the OpenFOAM package and self-similar solution of the problem, concerned to a point explosion in the gas-water mixture of the plane configuration, obtained by L.I. Sedov [11], was carried out, using the software implementation of this analytical solution [12]. Here it was assumed, that in a gas-water mixture the presence of liquid particles in the gas increases the inertia of medium, which remains homogeneous in density: \( \rho = \rho_g(1 + k) \), where \( \rho_g \) is the density of gas, and \( k \) is a positive constant. In [11], the expression was obtained for adiabatic index of a gas-water mixture \( \gamma \), defined as the ratio of heat capacities of mixture components. Self-similar solution of the problem [11] is obtained under the following initial conditions: \( \rho_0 = \rho_{g0}(1 + k) \), gas nitrogen with density \( \rho_{g0} = 0.0125 \text{ kg/m}^3 \), \( k = 10 \), \( \gamma = 1.1 \), energy of a point explosion \( E = 10 \text{ J} \). Initial values of pressure and temperature in undisturbed state: \( p = 0 \text{ Pa}, \ T = 0 \text{ K} \).

In the case of numerical simulation of the same problem using two-phase approximation with OpenFOAM package, the values of initial parameters close to the chosen for self-similar solution, were selected. The initial volume fraction of the gas nitrogen \( \alpha_{g0} = 0.99 \) corresponded to the initial density of the mixture \( \rho_0 = \rho_{g0}\alpha_{g0} + \rho_{l0}(1 - \alpha_{g0}) \), \( \rho_{l0} = 1000 \text{ kg/m}^3 \). On the left boundary of computational domain the time dependences of pressure \( p(t) \) and temperature \( T(t) \) were set as a boundary conditions in accordance with data, obtained from the analytical solution [11] for the coordinate, located from the explosion point at \( x = 0.04 \text{ mm} \).

In Fig. 2 the profiles for pressure \( p \) at the indicated times are presented. The solid line corresponds to the analytical solution [11] and the dashed line marks the numerical results obtained using OpenFOAM solver. Both solutions have a satisfactory agreement.

4. Numerical results

The results of numerical simulation the selected outflow mode are shown on Fig. 3 in the form of fields dynamics for velocity, pressure and temperature. In Fig. 3 at the time \( t = 20 \mu s \), as in experiment, the calculations show an intense expansion of the jet, while it reaches supersonic
Figure 2. Comparison of calculated profiles for pressure $p$ at the time moments $t$ ($\mu s$). Solid lines – the analytical solution for Sedov’s problem of a point explosion in the gas-water mixture [11] in the plane case, dashed lines – the numerical result of the same problem, obtained by using two-phase approximation of the OpenFOAM software solver.

outflow velocities $|\vec{v}| \approx 1000$ m/s. The barrel shock is formed along the boundary of expanding supersonic jet, with its reflection from the symmetry axis, the normal shock wave (Mach disk) is formed, which is the boundary zone between the regions of supersonic and subsonic flows. The main gas flow is formed along the lateral boundary of the jet, which is also characterized by a supersonic outflow regime. With the passage of time ($t = 60 - 100$ $\mu s$), the supersonic outflow regime is maintained along the outer region of the jet. Interaction of a high-speed flow with a weakly perturbed zone adjacent to it leads to curvature of gas trajectory and development of Kelvin-Helmholtz instability, which is accompanied by generation and development of vortex zones. At the time points $t = 60$ and $100$ $\mu s$, the process of forming a series of toroidal vortices that affect the twisting of jet towards the outer region is shown. Formation of a series of vortex zones near the axis of symmetry in gas, surrounding the jet, leads to appearance the oscillating form of the main jet flow with preservation of cavity inside the jet. The insignificant vapor condensation obtained in the calculations under conditions of equilibrium state in the low-pressure zones does not affect the process of jet evolution. Over time the jet flow forms a sequential series of acoustic wave pulses with periodic structure in initially unperturbed gas region, which can be a source of pulsations, observed in experiments [2], [3].

5. Conclusion
On basis of spatial axisymmetric two-phase model in one-velocity, one-pressure, two-temperature approximations, which take into account heat and mass transfer processes of evaporation and condensation, a non-stationary process of outflow from high-pressure vessel through a thin nozzle of water fluid, initially in near-critical state, is investigated. The numerical implementation of constructed model was made in reactingTwoPhaseEulerFoam solver of OpenFOAM library modification.

The reliability of used numerical method was shown by comparing the analytical exact solution and the numerical approach using OpenFOAM package, as applied to L.I. Sedov problem about point explosion for the case of plane configuration in gas-water medium.
Figure 3. Evolution of the calculated distribution of pressures $p$, mass velocities $v$ and temperatures $T$ in the process of hot vapor outflow through a thin nozzle at the indicated times $t$ ($\mu$s).
The performed numerical studies of supersonic outflow modes from the near-critical state of intensely expanding jet revealed the conditions for generation of barrel shock with formation of Mach disk. It is noted, that appearance of low-pressure zones is accompanied by vortex generation and twisting of the jet towards outer region. It is shown, that the further development of the main jet flow is influenced by formed groups of toroidal vortices, which lead to a sequence of wave pulses in the gas region (to acoustic pulsations) preceding the main jet.

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