Simulating gas (vapor) outflow into a liquid

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Abstract. In this paper, an axisymmetric problem of gas outflow from a pipe end to an area of high density (two-phase mixture) is considered. Simulation of the two-phase coolant outflow without phase transition is carried out using a two-velocity model, solved by the LCPFCT software package [1]. Cross-verification is performed with the results of calculation obtained by the OpenFoam software [2] using the VOF method for the approximation of the single-velocity model of a two-phase compressible medium. Using various numerical programs and various physical models of a two-phase medium gives a more complete understanding of the occurring processes.

1. Introduction
In order to prevent accidents in the steam generators of liquid metal nuclear reactors, there is a necessity of adequate simulation of processes of rapid depressurization of vessels with gas (steam) at high pressure with subsequent non-steady gas outflow into the liquid volume. Similar problems arise, for example, in the study of non-standard operation modes of pneumatic systems in naval technology [3], and depressurization of underwater gas pipelines [4].

The specific features of numerical simulation of such problems result from the need to take into account a complex of interrelated physical phenomena: the conjugate process of wave generation in an external medium and in high-pressure vessel, nonstationary gas outflow, and the process of liquid displacement by a gas.

In the calculation of the dynamic behavior of a two-phase medium, the adequate simulation of interfacial interaction is very important. In the absence of phase transitions and at a neglect of the processes of fragmentation and coagulation in the simulation of the dynamics of a two-phase mixture, the dimensions of droplets and bubbles may be assumed unchanged. This approximation is used in many quasi-one-dimensional thermohydraulic codes (for example, [5]). That is, with a pressure decrease, the gas content of the mixture increases not due to an increase in the bubble radius, but due to the increase in their number. In [6], using a two-fluid model, the two-phase mixture outflow to the high-density medium was numerically simulated and compared with an asymptotic simplified model of the gas cavity growth in the liquid volume.
2. Computing technique

Figure 1. Computational domain for two-velocity model (a) and that for OpenFoam, side view (b), three-dimensional view (c). a: $k$ – Cauchy – Lagrange boundary condition [7]; $P_a$ – the free flow boundary condition; $l$ – the channel length; $r_1$ – the inner radius; $r_2$ – the outer radius, b: $P_{in}$ is constant pressure BC, $w$ is the wall-type condition, and $P_a$ is the free flow BC at constant pressure.

In this paper, we consider the axisymmetric problem of the outflow of a two-phase mixture from the pipe end to the high-density area (the two-phase mixture with small volume gas content). Problem solution implied cross-verification of two different programs by different physical media models.

In the first case, the two-phase coolant outflow was simulated using the two-velocity and two-temperature model [8]. At that the model equations were solved using the LCPFCT software package [1]. This package uses the finite volume method along with the flow correction method (FCT). Simulation of the gas-liquid mixture outflow from the vessel required simultaneous calculation of the flow in the vessel, in the pipeline and in the outer region. A simplified "inlet area model" [7, 9] was applied to conjugate the flow in the vessel and in the pipeline. In this model, an incompressible medium motion is described by a one-dimensional Cauchy-Lagrange integral and allows calculating the pressure and velocity of a fluid at a known pressure in the vessel. When calculating the interfacial friction, it was assumed that the dispersed phase has the form of a sphere (droplets and bubbles).

The two-velocity and two-temperature model of a compressible medium without phase transition was described in detail in [10, 6]. Figure 1(a) presents an axisymmetric computational domain. In the pipe with the internal radius $r_1 = 20$ mm and the length $l = 100$ mm there is a two-phase medium with a large volumetric gas content (0.99) at a pressure of 10 MPa (Fig. 1(a),
red area). The external medium is filled with a two-phase mixture with low gas content (0.1) at a pressure of 0.1 MPa (Fig. 1(a), blue area). At the outer boundary, the free-flow boundary condition $P_a$ was set at constant pressure. At the tube inlet, a condition of “Cauchy-Lagrange” – $k$ \cite{7} was set. The chosen model mixtures were the air-water mixture and the air-lead mixture. The parameters of gas corresponded to those of air at a temperature of 200 $^\circ$C. The fluid parameters corresponded to the water parameters at a temperature of 100 $^\circ$C and the liquid lead at a temperature of 377 $^\circ$C \cite{11}. There was no heat exchange between the phases.

Figure 2. The distribution of the volume fraction of water calculated from the two-velocity model (a,b,c) and the non-slip phase model with the VOF method (d,e,f) at different times (a,d - 0.3 ms; b,e - 0.75 ms; f,c - 1.2 ms), (a,b,c): white color $\alpha \approx 1$, blue color $\alpha \approx 0$, (d,e,f): blue color $\alpha \approx 1$, red color $\alpha \approx 0$

In the second case, the problem was solved by the VOF method \cite{12} using the OpenFoam package. For a single-fluid model, the problem formulation included the Navier-Stokes equations, the continuity equation, and the transport equation for the volume fraction of a liquid. The local properties of the simulated fluid were calculated for the weighted average volume of fluid and gas properties. To calculate the surface tension forces, the Continuum Surface Force (CSF) model \cite{13} was used. In this model, the surface tension forces were reduced to a bulk force that is nonzero only in the vicinity of the interface.

Figure 1(b) shows the calculation area performed in OpenFOAM. The implementation of the axisymmetric problem on the 3D solver of the compressible InterFoam in OpenFOAM is performed using the computational domain in the form of a sector with a small angle ($\theta = 1^\circ$) (Fig. 1(c)). The parameters of the computational domain completely repeat the computational domain performed on the LCPFCT solver except for the “Cauchy-Lagrange” condition. Instead of the “Cauchy-Lagrange” condition, a large volume was installed at the entrance to the pipe (Figure 1(b)) with the boundary condition for free inflow at constant pressure $P_{in}$.
3. Results

Figures 2–3 show a comparison of the calculation results for air outflow into water and lead, respectively, using a two-velocity model and a non-slip phase model with VOF method. In the first case (Fig. 2,3(a,b,c)), as a result of gas and liquid simulation by two interpenetrating continua, a strong "smearing" of the interface is observed. In the second case, a gas bubble of complex shape is formed (Fig. 2,3(d,e,f)). It may be noted that the flow rate in the two-phase air–water system is substantially higher than in the air–lead system. So, for a two-velocity model for the air-lead system (Fig. 3(a,b,c)) the boundary is less clear than for an air–water system (Fig. 2(a,b,c)). A non-slip phase model model with VOF method is characterized by the appearance of a complex interface. For the air-to-water system (Fig. 2 (d,e,f)) the surface becomes close to spherical. In the air–lead system (Fig. 3 (d,e,f)) the interface is similar to the "mushroom" shape, which is determined by the wave pressures in the gas phase. Consider the air–lead pressure profile for the two-velocity model (Fig. 4(a)) and for the non-slip phase model with VOF method (Fig. 4(b)). In the first case, a smooth pressure decrease is observed for the two-velocity model. The VOF method is characterized by an abrupt change in pressure. At that the first jump occurs as a result of the critical outflow of the gas, and the second one results from the existence of the interface.

When solving this problem, the use of various numerical programs and various physical models of a two-phase medium, each having its advantages and disadvantages, gives a more complete understanding of the occurring processes. At the same time, the relevance of program verification in field experiments remains. The two-velocity model is suitable for problems where one of the phases is in a dispersed state and the phases are sliding relative to each other. VOF-method gives more adequate results in problems with one phase displacement by another phase, since the presence of a complex interface requires prediction of its evolution.
Figure 4. Pressure profile for the air–lead system is a two–velocity model (a) and a non–slip phase model with VOF–method (b) at different times (1 – 0.3 ms, 2 – 0.75 ms, 3 – 1.2 ms)

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