Dynamics of gas phase concentration in SPH

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Abstract. Various approaches are considered in the method of smoothed particle hydrodynamics (SPH) for calculating the volume concentration of gas phase in a liquid during the rarefaction or destruction. A scheme for calculating the concentration of gas phase, consisting of three stages, is proposed. At low concentrations, the calculation is carried out according to the full model, which includes the laws to describing the concentration dynamics. At high concentration the simplified model is used, when the change in concentration is determined by the dynamics of liquid. When the maximum concentration is reached, corresponding to a single particle without neighbors, the rate of concentration growth is fixed and the further development of the process is governed by inertia.

1. Introduction

Method of smoothed particle hydrodynamics (SPH) [1] belongs to purely Lagrangian methods and allows us to conduct a numerical study of fluid flow in a strongly deformable of calculation domain, in particular, when the medium is expanded or destroyed. In that case rarefaction resulting in scattering of SPH particles and empty areas occurrence of in the liquid, which in reality are filled with air or liquid vapor [2].

When modeling the dispersion of SPH fluid, various approaches can be used. In the single-phase model, the common equation of state for a fluid is as follows:

\[ p = B \left( \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right), \quad \rho \geq \rho_0. \]

A more correct approach is to take into account the gas phase. This can be done, assuming that the vacuum is instantly filled with gas. In this case, the dynamics of concentration of the gas phase \( K \) is completely determined by the dynamics of the liquid. The equation of state of a two-phase medium is modified as follows:

\[ p = B \left( \left( \frac{\rho}{\rho_0(1-K)} \right)^\gamma - 1 \right), \quad K = \begin{cases} 1 - \frac{\rho}{\rho_0}, & \rho < \rho_0, \\ 0, & \rho \geq \rho_0. \end{cases} \]  

In this approach, there is no inherent dynamics of gas phase, which could play a significant role in the decompression of the environment, or have its own characteristics associated with specific conditions. In a more complicated case, the dynamics of the gas phase is determined by specific laws, which may include the effects of diffusion, degassing, chemical reactions, etc. In the latter case, it is necessary to use multi-phase models.
A volcanic eruption process can be taken as an example, where degassing occurs in the initially compressed gas-saturated magma, bubbles form and grow, but their growth essentially depends on the viscosity [3]. A situation is possible in which the growth of bubbles is hindered, despite the continuing destruction of the medium. Therefore, in this case, it is necessary to separately take into account the dynamics of gas phase.

Thus, it turns out that in the SPH method there are two mechanisms of cavitation, the first one is associated with rarefaction of particles, and the second one with specific physical laws governing dynamics of gas phase.

2. Statement of problem
Consider a model problem of decompression of the liquid layer in a one-dimensional formulation. A liquid layer at pressure \( p = 150 \text{ atm} \), uniformly seeded with air bubbles, occupies space of length \( L = 5 \text{ cm} \). Initial radii of the bubbles are \( R_0 = 5 \mu\text{m} \), and pressure in the bubbles is equal to the liquid pressure. At the moment of time \( t = 0 \), the right boundary becomes free and the pressure at the boundary drops to atmospheric \( p_0 \text{ atm} \).

To describe the processes taking place, a well-known Iordanskii – Kogarko – van Wijngaarden (IKW) [4] model is used. It consists of the equations of gas dynamics, which in conventional notation, have the form:

\[
\begin{align*}
\frac{d\rho}{dt} + \rho \frac{dv}{dx} &= 0, \\
\frac{dv}{dt} + \frac{1}{\rho} \frac{dp}{dx} &= 0,
\end{align*}
\]

Rayleigh equation for the dynamics of a single bubble:

\[
R \frac{d^2R}{dt^2} + \frac{3}{2} \left( \frac{dR}{dt} \right)^2 = \rho_0^{-1} (p_g - p),
\]

Tait equation describing the compressibility of the liquid phase:

\[
p = p_0 + \frac{\rho_0 c_0^2}{n} \left( \left( \frac{\rho}{\rho_0 (1 - K)} \right)^n - 1 \right),
\]

and the following relationships:

\[
\rho = \rho_0 (1 - K), \quad K = \frac{K_0 \rho}{\rho_0 (1 - K_0)} \left( \frac{R}{R_0} \right)^3, \quad p_g = p_0 \left( \frac{R}{R_0} \right)^{3\gamma}.
\]

Here \( K \) is the volume concentration of gas phase, \( R \) - radii of bubbles, \( \rho_0 \) - density of the liquid phase, \( p_g \) - pressure in bubbles, \( p \) - pressure in medium, \( \rho \) - average media density, \( c_0 \) - the speed of sound in a liquid, \( p_0 \) and \( K_0 \) - atmospheric pressure and initial concentration.

Each particle in SPH method is associated with a certain amount of the simulated medium, we assume that the particle also contains a certain number of gas bubbles with radius \( R \) [5]. The dynamics of gas phase at low concentrations, when the bubbles can be considered spherical, can be described by the Rayleigh equation (3). At high concentrations (in our case at \( K > 0.2 \)), we assume that the pressures in the gas and liquid phases have leveled off and use the relations (1).

With this approach, the parameters associated with gas phase can be calculated in different ways. First, in accordance with the used model of the dynamics of gas phase, and second, the value of any function specified in SPH particles is calculated in accordance with the interpolation formula of the method:

\[
f(r) = \int W(r', h) dr'
\]

where \( W \) is the smoothing core, \( h \) - the width of the kernel.

In the present study on decompression of a liquid with gas microbubbles compares the results obtained with both approaches.

3. Results of numerical simulations
At the initial moment of time, the right boundary of the fluid becomes free and decompression wave propagates through the fluid. Figure 1 shows the pressure distribution in the medium and gas phase for a time instant of 10 \( \mu \text{s} \), during which the wave propagated in the layer to \( \approx 1.5 \text{ cm} \). Fluctuations of
bubbles behind the wave front around a new equilibrium state result in pressure pulsations, which are clearly visible in the graphs. At the free boundary, the fluid particles acquire certain velocities and the medium begins to expand. It can be seen from the volume concentration (figure 2), that in a narrow layer the parameters corresponded to different particles have a significant scatter.

![Figure 1. Pressure of liquid and gas on t = 10 μs.](image1)

![Figure 2. Concentration of gas phase on t = 10 μs.](image2)

Note that if in the rest of the domain the concentration of gas phase in the particles calculated using the IKW model does not differ from the interpolated value (5), in contrast with the expansion region. In some cases, the difference may be important, say, when determining the maximum concentration value in the domain. It is clearly seen that such values must be searched for individual particles without interpolation.

After the decompression wave passes through the entire region, the liquid layer acquires certain speed and moves to the right almost as a whole. This follows from the distribution of the mass velocity in the layer shown in figure 4. At the left boundary, a rarefaction is also observed, since the boundary naturally remains fixed. The distribution of the volume concentration at the time 100 μs is shown in figure 3. It is also well seen that the interpolated values of the concentration differ from the values in the individual particles.

![Figure 3. Concentration of gas phase on t = 100 μs.](image3)

![Figure 4. Velocity on t = 100 μs.](image4)
At later times (figure 5), there is a strong rarefaction of particles in this region and the formation of gaps between them. It should be noted that the graph in the figure is plotted not as line but by points, each of which corresponds to a particle. If particles are close to each other, the gaps are not visible at this scale, while in the rarefaction zone they can be seen as dots on the graph (figure 5). From the point of view of the SPH method, this corresponds to a decrease in the number of neighbors for each particle, up to the loss of all neighboring particles.

Figure 5. Concentration of gas phase on $t = 0.01$ s

In this situation, the density in the particle reaches its theoretical minimum, which corresponds to the maximum possible value of $K$ according to the model (1). In this case, it is more correct to speak of liquid drops flying in the surrounding space. And, from this point of view, $K$ should continue to grow, as the particles fly away from neighbors. According to model (1), growth stops at the maximum value. Figure 6 shows the dynamics of the concentration of gas phase in a particle near the left boundary. This effects can be taken into account by putting a constant value of the growth rate $K$ when the maximum concentration is reached. In fact, this means that a further increase in concentration occurs at a constant rate, by inertia. On the other hand, when an SPH particle loses all its neighbors, its further motion also occurs by inertia, since the forces from the other particles are zero.

Conclusion
This study proposes an efficient scheme for calculation for expansion and destruction of a liquid during decompression using the SPH method. The calculation of the volume concentration of gas phase is divided into 3 stages. At low concentration, the calculation is carried out according to the full IKW model (2–4), with possible account for additional effects, such as diffusion or chemical reactions. At high concentration, up to the limiting one, a simplified model (1) is used. When the maximum concentration is reached, one can take $\frac{dK}{dt} = \text{const}$. The proposed model allows to simulate the concentration of the gas phase in the entire possible range of values.

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