Simulation of interphase dynamic exchange in a heterogeneous natural system

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Abstract. A model of hydrodynamics of a two-phase liquid-solid system is formulated, in which forces of interphase dynamic interactions are taken into account. A scenario on distributions of insoluble solid particles emerging from an area source at the bottom of a lake in a stratified medium is considered. A calculation is performed in a three-dimensional statement taking into account the basic parameters of Lake Baikal. The results of the numerical simulation under winter conditions have shown that the two-phase system has a complex behaviour in space and time. The presence of solid particles strongly affects the hydrodynamics of the system and serves as a trigger for deep convection.

1. Introduction

The underwater gas outlets in Lake Baikal have been known since the time of its first research. The formation of holes in the ice cover, gas bubbles frozen into the ice, noisy exits of the flammable gas in violation of the ice integrity gave rise to many legends in their time.

The first evidence of the existence of gas hydrates at the bottom of the lake was obtained in the summer of 1978 by the staff of the VNIIGAZ Institute when studying the bottom sediments in Southern Baikal. The first publication on the possibility of existence of gas hydrates in the sediments of the freshwater lake appeared in 1980. Since then the studies of the “gas content” of the lake have developed in a wave-like manner corresponding to the current situation and reaching a natural maximum after expeditions with the help of underwater vehicles “Mir” in 2008-2010 [1-2]. Then it was possible not only to confirm the presence of hydrates in the sedimentary accumulations, but also to witness the surprising fact of superficial occurrence of sufficiently extensive hydrate fields in several areas of the lake.

The specificity of Lake Baikal lies in the fact that because of large depths (maximum of more than 1600 m), gas hydrates can be stored in the water without decomposition not only on the bottom at high pressure, but also within the water column, below a depth of about 380 m [1]. In full-scale experiments performed on board the “Mir” station, it was shown that hydrates can also be formed from gas and water inside the water column and exist not only in the form of crystals but also as hydrate powder and hydrate foam [2].

In this context, the necessity arises of studying the behaviour of multiphase media in the natural conditions of deep water bodies. This is especially important given the fact that the lake contains more than 23,000 km³ of clean drinking water, and by the decision of UNESCO it is a World Heritage site.

Studies of multiphase systems are widely reflected in the scientific and technical literature. Classical theoretical foundations can be found in [3]. Most of the research is devoted to closed volumes, such as, for example, chemical reactors, pipelines of various diameters, etc. However, it is obvious that
there is a difference between a closed volume and open natural environments, such as oceans, seas, and large deep water objects, where there are also underwater gas outlets and hydrate deposits. Such a difference, if any, should be studied. This paper continues the research cycle [4-7] devoted to such problems.

2. Some physical facts
Hydrate is a crystalline structure similar to snow. The ideal formula for methane gas hydrate has the form $\text{CH}_4(\text{H}_2\text{O})_{\text{ss}}$, and the molecular weight is 121.3 g / mol. The density of hydrate is 0.9 g / cm$^3$, the gas saturation is $G = 13.2\%$. Since gas hydrate is lighter than water, it will float up in water. Causes of gas hydrate entering water can be, for example, landslides and earth movements due to earthquakes.

During the ascent, two processes take place with the crystals: dissolution and dissociation. These two processes have completely different nature with respect to the internal stability of the crystals. In the first stage, when lifting to a depth of about 380 m hydrate is internally stable, but under the influence of the surrounding water environment, the molecules are washed out from the surface of the crystals. In this stage of the lift the hydrate mass is practically unchanged, since its dissolution rate is small, only a few mm/year.

At depths of about 380 m, gas hydrate begins to dissociate into gas and water. This is a different process, it occurs due to the fact that the hydrate becomes internally unstable. There is a rupture of the internal bonds in the molecules themselves resulting in a phase transition. This process is quite fast. At lower depths, gas hydrate can no longer exist in the equilibrium state. However, some of it can get to the surface before decomposing. This depends on how large the crystals of the pop-up fragments were originally. Note that the processes of decomposition and formation of gas hydrate occur with the absorption and release of heat, which affects the thermodynamics of the system.

There is also another specificity of the lake, also associated with its depth. It is a change in the temperature of the maximum density, which regulates the processes of natural and (forced) vertical water exchange. The fact is that due to the influence of pressure the temperature of the maximum density decreases from 4 degrees C on the surface by 0.21 degrees every 100 m. As a result, twice a year in spring and autumn, the natural mixing processes in the lake are limited to the upper 250-300 meters, without affecting the rest of the water column. Depths between 250 and 300 m are in some sense critical: here the slightest changes in the heat content can cause significant hydrodynamic effects due to the decomposition of hydrates if they are there, because decomposition occurs with the exchange of heat with the environment.

However, purely dynamic mechanical processes can move the water masses with their properties in such a way that in the adjacent vertical layers the temperature stratification will change to the opposite. This can happen when the temperature in situ passes through the maximum density temperature at this depth. This can cause forced convection in deep layers and, therefore, "refresh" the deep waters. This case without mass transfer between the phases in the system is considered here.

3. Mathematical model
Mathematical modelling provides us with such a possibility as different model formulations studying certain aspects of the behaviour of the physical system. In this paper, we restrict our consideration to the case of only the hydrodynamic aspects of modeling a two-phase system "liquid-solid particles" in a three-dimensional setting. The mass exchange between the phases, the thermodynamic and chemical processes are not taken into account here in order to consider separately the dynamic phase interactions.

The mathematical model for the multiphase flows is formulated in the so-called Euler-Euler statement. The phases are assumed to be interpenetrating continua. The volume fractions of each phase in a unit volume of a two-phase system are designated as $\epsilon_i ; k = \{l, h\}$, and $\epsilon_l + \epsilon_h = 1$. It is believed that water is a carrier medium and $\epsilon_l \subset \epsilon_h$. In this technique, there is no need to monitor the detailed
account of the boundaries between the phases. For each phase, a complete set of equations for the momentum and the continuity equation are solved. The phase combination is achieved by means of a common pressure for the two phases and a description of their interfacial exchange.

We consider two systems of equations of conservation of mass and momentum for two media, water-solid particles. In this paper, as solid particles we will consider crystals of matter of specified sizes that are not subject to any changes during the process, and their true density is \( \tilde{\rho}_h = \text{const} \).

The continuity equations for describing the mass balances are:

\[
\frac{\partial (\rho_k u_k)}{\partial t} + \frac{\partial (\rho_k u_k u_k)}{\partial x} + \frac{\partial (\rho_k v_k v_k u_k)}{\partial y} + \frac{\partial (\rho_k w_k w_k u_k)}{\partial z} = 0, \quad k = l, h.
\]

The equations for the conservation of angular momentum have the form:

\[
\frac{\partial (\rho_k v_k)}{\partial t} + \frac{\partial (\rho_k u_k v_k)}{\partial x} + \frac{\partial (\rho_k v_k v_k)}{\partial y} + \frac{\partial (\rho_k w_k v_k)}{\partial z} = -\varepsilon_k \frac{\partial p}{\partial x} \pm F_x + \rho_k F^C_x + \rho_k D, (u_k),
\]

\[
\frac{\partial (\rho_k w_k)}{\partial t} + \frac{\partial (\rho_k u_k w_k)}{\partial x} + \frac{\partial (\rho_k v_k w_k)}{\partial y} + \frac{\partial (\rho_k w_k w_k)}{\partial z} = -\varepsilon_k \frac{\partial p}{\partial z} \pm F_z + \rho_k F^C_z + \rho_k D, (w_k).
\]

Here the indices \( h, l \) denote the solid and liquid components of the system; \( \rho_k = \varepsilon_k \tilde{\rho}_k \); \( \tilde{\rho}_k \) are the true densities; \( \tilde{\rho}_h < \tilde{\rho}_l \); \( F^C_k \) is the operator describing the components of the Coriolis force. The only difference between these systems is the different signs in the terms describing the force interactions. The positive sign is in the light phase, and the negative one is in the heavy phase. The buoyancy effect leading to the slip of the light phase with respect to the heavy phase is the result of combining the two phases at the same pressure. The second-order operator \( D \) describes the turbulent diffusion processes. In this version of the model it is the same for the water and admixture.

The interfacial dynamic exchange is usually described by parameterizations. Typically, three components of the interaction forces are considered: the drag force, the added mass force, and the lifting force:

\[ F = F^d + F^a + F^l. \]

The drag force is the largest contributor, and so only it is often taken into account:

\[ F^d = -\varepsilon_h C_f \tilde{\rho}_l |(u_h - u_l)|, \]

where \( C_f \) is a dimensionless drag coefficient, which depends on the parameters of solid particles.

While lifting, the solid particles are accelerated relative to the liquid. In this case, part of the surrounding water is also accelerated after the impurity. This additional force is called the "added mass force" and is calculated by the formula

\[ F^a = \varepsilon_h C_a \tilde{\rho}_l \frac{d(u_h - u_l)}{dt}. \]

The coefficient \( C_a \) corresponds to the volume fraction of the liquid which is accelerated by the admixture.
In addition, one more component is the lifting force (Magnus force). If a particle with a solid shell moves in an inhomogeneous liquid, the flow of the liquid can cause the particles to rotate which, in turn, can create an additional force of interaction perpendicular to the main direction of motion:

$$F^m = c_n C_R \rho \left( u_n - u_i \right) \times (\nabla \times u_i).$$

To solve the systems of equations described above, numerical algorithms constructed on the basis of the variational approach and the splitting technique with the use of discrete analytical approximations with adjoint integrating factors are developed.

4. Numerical simulation for liquid-solid system

A numerical experiment simulates the propagation of insoluble solid particles from an area source located on the bottom in a stratified lake environment. The true particle density is constant and equal to that of methane hydrate.

A winter scenario is considered. The boundary conditions at the surface take into account the presence of ice cover. To the system of equations (1) - (2), we need to add an equation of temperature and an equation of state for the true density of water:

$$\rho_c \frac{dT}{dt} = \rho D_T(T) + q_T,$n\frac{\hat{\rho}}{t} = f(T, p, S_n),$$

where $\rho c_p = \sum_{k=1,2} c_k$. The water density is also the desired function depending on the temperature, pressure, and salinity. In this case, the latter is considered a constant. Here $q_T$ is not related to the heat transfer between the phases, but describes the volume absorption of the heat coming through the surface of the lake. In the short scenario for the winter season with ice cover under consideration these are small values.

Figure 1. Bottom topography.

The initial distribution of the temperature is taken uniform in horizontal directions in correspondence with a real vertical distribution of the temperature at a site in Southern Baikal in winter. This distribution is characterized by a strong stable stratification with an inverse temperature profile from 0°C at the surface to the mesothermal maximum layer where the warmest water of 3.5-3.6°C is located.
The solution domain is a three-dimensional volume with real coastal outlines and relief of the bottom of the southern tip of Lake Baikal. The area source is located approximately in the middle of the domain at depths of about 1250 m (Figure 1).

Analysing the results of the scenario, we see that the system demonstrates a complex behaviour in space and time. Figure 2 shows the initial ascent period. The impurity reaches the surface in 3 hours (Figure 2, a). On the sides of the rising stream, currents of the reverse direction are formed (Figure 2, b). When the hard boundary of the ice cover at the surface is reached, the water masses slightly spread out to the sides, and then begin to fall down.

![Figure 2](a) ![Figure 2](b)

**Figure 2.** Snapshot of the vertical distribution through the centre of the area source in a section across the lake: volume fraction of the solid phase and velocity vector (a) in 3 h and (b) in 4 h.

![Figure 3](a) ![Figure 3](b)

**Figure 3.** The same as in Figure 2, but (a) in 5 h and (b) in 6 h.

The further behaviour of the system can be seen in Figures 4 and 5 where the temperature isolines are shown. After the first portions of the raised water collapsed, the cold water begins to fall along the sides of the main stream (Fig.3), which leads to the renewal of the bottom waters (Fig.4,b). This is a
very remarkable fact, since Lake Baikal, due to natural convection, can renew the water only to depths of about 300 m.

![Figure 4](image)

**Figure 4.** Snapshot of the vertical distribution through the centre of the area source in a section across the lake: isolines of temperature and velocity vector (a) in 3 h and (b) in 6 h.

![Figure 5](image)

**Figure 5.** The same as in Figure 4, but (a) in 11 h and (b) in 20 h.

The dynamical behaviour of the system discussed at the end of Section 2 is clearly seen in Figure 5. The renewal of deep water occurred as a result of the emergence of solid particles and the subsequent mechanical movement of the water masses. The resulting system of currents led to a change in the stratification of the water column. This triggered deep water convection.

5. **Conclusions**

A model of hydrodynamics of a two-phase liquid-solid system has been formulated, in which forces of interphase dynamic interactions are taken into account. A scenario on distributions of insoluble solid particles emerging from an area source at the bottom of a lake in a stratified medium was considered. A calculation was performed in a three-dimensional setting taking into account the basic
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