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Modeling of Phase Transitions in Hydrodynamics

A method of direct numerical simulation for some heterogeneous fluid dynamics with take of phase transitions will be presented. It is supposed that the fluids are compressible and inviscid (non-viscous). Heterogeneities of the fluids are considered as small drops or particles of one fluid within other fluid. Total number of the drops can be large enough and the drops may have phase transitions. Thus, simulations of the main fluid (or gas) with small transited drops dynamics are discussed. These are dynamics of multiphase flows really. Therefore it is possible to use general multiphase flow models in the case. But standard multiphase equations are not complete as a rule and various physical experiments are necessary for solving of the problem for concrete heterogeneous fluid dynamics. The situation is more difficult whenever phase transitions are possible.

Presented method is a combination of Harlow's particle-in-cell method and Belotserkovskii's large particles method (see, for example, [1]). The method is based on a discretization of conservation laws for masses, momentums, and energies in integral forms. The discretization is natural and numerical simulations are realized as direct computer experiments for the dynamics of main fluid together with transited drops without use multiphase flows approach. The method seems to be much more adequate to the mechanical and mathematical essence of the dynamics, because conservation laws are correct on the discrete level at least.

The method is designed to computer modeling of following physical processes. Let us consider graphite particles distributing uniformly in some fluid. More exactly there is medium with graphite particles and the medium can be considered under high pressure as "fluid" with corresponding state equation. Inducing conical shock waves in the heterogeneous medium, it is possible to observe dynamics and phase transitions of the graphite particles in computer experiments by the method, where the transitions are realized if the pressure or temperature is more (or less) than the critical pressure or temperature by relevant phase diagrams. Results of the computer experiments are in agreement with results of physical experiments. The results are greatly depending on density of graphite particles and intensity of the shock waves.

The method seems to be perspective for numerical simulations of other absorption and diffusion processes in complex fluid and plasma dynamics (see, for example, [2]).

[1] Belotserkovskii O. M. and Davydov Yu. M., The method of large particles in gas dynamics. Numerical experiments. — Moscow: Nauka, 1982.

[2] Boyko S. B., Mischenko V. V., and Sandrakov G. V., // J. Computing and Applied Math. — 2007. — **95**, N 2.