Computational Fluid Mechanics with Phase Transitions by Particle Methods

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Abstract—**A computational method of simulations for processes of heterogeneous hydrodynamics with take of phase transitions will be discussed. The method is based on relevant approximation of conservation laws for mass, momentum, and energy in integral and differential forms. The time and spatial approximation is natural and numerical simulations are realized as direct computer experiments. It is supposed that the fluids are compressible and non-viscous. Heterogeneities of the fluids are considered as small drops or particles of one fluid within other fluid. Total number of the drops may be large enough and the drops may have phase transitions. Therefore, simulations of the main fluid with small transited drops dynamics are considered. The particle dynamics will be modelled as in the particle-in-cell method, and in the main fluid as in the large particle method. This approach makes it possible to simulate phase transitions under certain assumptions about heterogeneous fluids. The calculation algorithm of this method is implemented as a computer simulation of the dynamics of a multiphase carrier fluid containing particles that can undergo, for example, graphite-diamond phase transitions. Such transitions are modelled on the basis of the theory of phase transformations and the laws of thermodynamics. In fact, the method is a combination of the Harlow's particle-in-cell method, Belotserkovskii's large particles method and Bakhvalov's homogenization method. A modification of this method has also been developed to take into account the effects of viscosity when simulating the dynamics of a multiphase fluid in porous media. A model of the motion of such a liquid in a porous medium is obtained by freezing the motion of particles of the corresponding size in the presented method. The method will certainly be promising for numerical simulations of absorption and diffusion processes in complex fluids with phase transitions.**

Keywords—conservation laws; particle-in-cell; large particles; approximation; homogenization; multiphase models; porous media.

I. Introduction

Mathematical and computational modeling plays a significant role in understanding the phenomena and processes that are investigated in modern physics and chemistry. The modeling can help interpret and even prediction new phenomena. Researching the physical and chemical processes which are in heterogeneous media at large speeds, high pressures and energies in the field of phase transitions, it is required to have accurate values of pressures, energies and velocities arising at various points of these substances at suitable times. Such values are significant in order to understand the state of media and the phase transitions that have taken place. The determination of such values is possible on the basis of modeling of nonlinear hydrodynamic processes in heterogeneous fluids.

The significance of this problem is due to the intensive development of the branches of physics and chemistry associated with the study of dynamic processes occurring during pulsed loading and the passage of shock waves in metals, polymers and heterogeneous composites [1]. The study of such processes is necessary for the development of new technologies that use the methods of pulsed and shock loading, which make it possible to synthesize new substances. The formation of new substances, their modifications and phases is associated with physicochemical processes initiated at high pressures and energies. The calculation of such wave processes is complicated, since these physicochemical processes strongly affect the behavior of the initiating waves. In addition, phase transitions under the action of waves loading can lead to multi-front waves. To analyze these processes, the development of mathematical models are necessary, taking into account the basic principles of the theory of phase transformations, and the construction of highly efficient computational method and algorithms.

Thus, the computational method of simulations for processes of heterogeneous hydrodynamics with take of phase transitions will be discussed. It is supposed that the fluids are compressible and non-viscous. Heterogeneities of the fluids are considered as small drops or particles of one fluid within other fluid. Total number of the drops may be large enough and the drops may have phase transitions. Therefore, simulations of the main fluid with small transited drops dynamics are considered. In fact, the method is a combination of the Harlow's particle-in-cell method [2], large particles method [3] and homogenization method [4] that is based on conservation laws.

II. Methods

Actually, there are no real models for processes describing the behavior of heterogeneous materials at high pressure and energy in the field of phase transitions in the available literature. The problem of the models, taking into account the basic provisions of the phase transition theory, was posed by V. Yudovich as one of

the main problems of mathematical physics. This problem is not solved here, but a possible approach will be discussed for calculating the parameters of heterogeneous media at large speed, high pressure and energy in the field of phase transitions. The approach is based on an approximation of conservation laws for mass, momentum, and energy of fluids and performing simulations on relevant time intervals [5]. Initially, such an approach to this problem was proposed in [6].

An alternative approach to this problem is known, which is based on the concept of multiphase continuous media. In the case, the assumptions of a multi-speed continuum and interpenetrating motions of the components are accepted when deriving multiphase equations for suitable models. In a sense, this concept means the simultaneous presence of several materials at each point of the space under consideration; further details can be found in [1]. Also, the general multiphase equations for such multi-speed continuous media are not closed and contain indefinite terms. In such equations, for example, the terms of describing the redistribution of energies between phases during the development of the dynamics of multiphase media are not definite. Various physical experiments are necessary for solving of the problem in concrete cases. The situation is more difficult whenever phase transitions are admissible.

For the problems of diffusion and elasticity dynamics in heterogeneous composite media, there is a rigorous mathematical approach leading to multiphase homogenization models, which was originally presented in [7]. In the multiphase models, the media are not considered as several materials at each point of the space simultaneously. In these results, the solutions to the relevant multiphase equations for each phase are restrictions on the corresponding phase that can interact through the interchange terms. Such interchange terms are defined explicitly and so the problem of describing the redistribution of energies between phases does not arise when considering the dynamics of the multiphase media. This approach is also used in the method for mathematical modeling of structurally heterogeneous materials as heterogeneous fluids dynamics, which is presented here. The problem of describing energy redistribution between phases does not arise when this method is implemented. Energy redistribution in this method is performed through the assumption that the local pressure in each phase is the same. The assumption is natural according [1] and will be used in conjunction with particle-in-cell and large particles methods for the modeling of fluid mechanics with phase transitions.

Some trial and preliminary computer experiment results may be found in [8]. More details of the method and other modifications may be found in [8, 9]. It seems very important to realize the generalization of this method to be used for simulating the dynamics of a multiphase fluid in porous media in accordance with [8]. Alternative methods for the problems with relevant references may be found, for example, in [11] and [12].

III. Conclusions

Thus, the computational method of simulations for heterogeneous fluid dynamics with phase transitions is discussed. The method is based on approximation of conservation laws for masses, momentums, and energies in integral and differential forms. The approach is natural and numerical simulations are realized as direct computer experiments. The method seems to be much more adequate to the physical and mathematical essence of the dynamics because conservation laws are fulfilled on the discrete level. The calculation algorithm of this method is implemented as a computer simulation of the dynamics of a multiphase carrier fluid containing particles that can undergo, for example, graphite-diamond phase transitions. Such transitions are modeled on the basis of the theory of phase transformations and the laws of thermodynamics. A modification of this method has also been developed to take into account the effects of viscosity when simulating the dynamics of a multiphase fluid in porous media. The discussed method will certainly be promising for numerical simulations of other absorption and diffusion processes in complex fluids and multiphase fluids in porous media.

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