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SIMULATION OF HYDRODYNAMIC AND ELECTROHYDRODYNAMIC FLOWS BY LATTICE METHODS

PhD Thesis

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INTRODUCTION

This work deals with the study of fluid flows in different hydrodynamic and electrohydrodynamic processes (detonation waves in a porous medium, mixing of detonation products, inception and development of the electric breakdown in liquids), and related instabilities. Fluid flows are simulated by the lattice gas and lattice Boltzmann equation methods, that are relatively new methods based on the solution of the kinetic equation for simple model system.

Macroscopic dynamics of fluid is the average result of motion of its individual molecules. Interaction between molecules specify the properties of substance. Thus, one can simulate the behaviour of interacting particles itself and obtain macroscopic quantities (density, mass velocity, pressure and temperature) by averaging. This approach underlies the molecular dynamics method. In this case, the discretization of a problem (individual particles) corresponds to the properties of real physical world. The number of molecules in virtually any real system is so great that the full-scale simulation is most likely impossible ("one needs a gram-molecule of computers in order to simulate a gram-molecule of substance"). Therefore, one have to restrict oneself to comparatively small systems with further extrapolation of the results obtained to much larger spatial and temporal scales.

The approach of traditional hydrodynamics is, on the contrary, essentially macroscopic. The numerical methods consist of the solution of partial differential equations discretized properly in space and time. The variables in this case are macroscopic quantities themselves.

Lattice methods lie in a sense between micro- and macroscopic approaches. One can name them mesoscopic. The theoretical basis of lattice methods is the fact, that macroscopic behaviour of a medium only slightly depends on the details of its microscopic structure. The particularities of the structure and interaction of particles affects only the transport coefficients (diffusivity, viscosity and heat conductivity). One can therefore choose very simple microscopic properties (that should significantly simplify the computations), and hope nevertheless to obtain on the macroscopic level an adequate description of real medium.

Lattice methods have common features both with the molecular dynamics (the dynamics of system of particles are considered, although they have extremely simple properties) and with the usual finite-difference methods (the space and time are discretized too).

Of course, there are no ideal computation method, each approach has advantages on a certain class of problems. Lattice methods are superior in the

computation of flows where the structure and interaction on a mesoscopic scale are essential. The simulation of such flows is a subject of this work.

Dissertation consists of five chapters.

In chapter 1, the overview of the Lattice Gas Automata (LGA) and the Lattice Boltzmann Equation (LBE) methods are given. Different modifications of the LBE method are presented (the isothermal model, the model with variable temperature and the model with interparticle interactions). Some test computations were carried out.

A possibility to apply the LBE method to solve parabolic and elliptic equations is shown.

In chapter 2, the simulation of convective detonation waves in a porous medium is presented. Fuel forms initially a film on the pore walls. Pores are filled with oxidizer. Fuel evaporated from walls burns instantly. Computations was performed by the LGA method with additional simulation of exothermal chemical reaction, friction against the porous bed and heat losses. Computed wave velocity and pressure profile are in good agreement with experimental ones.

The chapter 3 deals with the simulation of mixing in a two-component system due to development of the shear flow instabilities. Flow evolution for different initial geometry was considered. The results obtained were used to compute the time dependence of the electric conductivity of detonation products of heterogeneous HE. The dependencies obtained were compared with experiment. The qualitative agreement of the experimental and computation data was shown.

Further, the modification of the LBE method to simulate electrohydrodynamic (EHD) flows is presented (chapter 4). Several methods to compute the convective charge transport were considered. Theoretical values of the numerical diffusivity were compared with computation results. Development of EHD-flow in different geometry was studied. In two-dimensional case, the flow has oscillatory character caused by the charge injection in discrete lumps that reduce the electric field. As the voltage between electrodes is increased, the liquid flow instability emerges which breaks the flow symmetry.

At certain conditions, the emergence of a region of gas phase was observed in computations. Such a bubble was generated in the region of high electric field (near the tip) due to to electrodynamic cavitation — homogenous nucleation in the region of low (or negative) pressure. The density inside the bubble decreased by three orders of magnitude. The time of bubble development increased with the decrease of electric field, this effect was of the threshold character. The electric breakdown of bubbles generated can result in the breakdown of liquid

by the bubble mechanism.

In chapter 5, the propagation of streamers and the dynamics of the electric discharge channel in liquid were investigated for planar and cylindrical cases. Divergent shock waves were observed at the channel expansion due to energy release in it and at the supersonic propagation of the streamer tip.

The inner structure of the channel boundary was considered, the transition layer "liquid–plasma". The non-monotonic pressure variation across the boundary due to viscous tension was shown. Theoretical estimates of the pressure jump on the channel boundary and of the pressure peak inside the transition layer agree well with computation results.

In the Conclusions chapter, the main results are formulated.

The results obtained are published in [1–14].