Adiabatic expansion of Lennard–Jones matter into the liquid-gas region

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The purpose of this work is to study a fluid sample expansion into the unstable liquid-gas region under isentropic expansion. To achieve this goal, the LAMMPS code is used. The work exploits a simulation scheme that resembles experiments with shock tubes. The test sample, which is in a high-pressure state, is placed in front of substances (anvils) with a smaller dynamic impedance (normal density times normal sound velocity). After that, the simulation process begins, during which the propagation of a shock wave and a rarefaction wave is observed in the simulation cell. The program allows one record the state of the system at various moments, observe the wave velocities, and calculate all the necessary thermodynamic quantities such as density, temperature, and pressure. It is shown that when low-density barriers are placed, the sample is unloaded to a state corresponding to the position of the two-phase region. However, a homogeneous state does not have time to form. A complex wave flow is realized, which differs from the theoretical concepts following from the solution of the discontinuity problem. In the course of numerical experiments, it was decided to use substances with a low atomic mass to obtain low-density barriers with a high concentration of particles. This change will make it possible to reduce the influence of the porosity of the anvil, as well as to study in more detail the processes occurring at the interface of the sample and anvil. The paper will present the distribution profiles of various quantities in the process of adiabatic expansion and their theoretical analysis, as well as animations of the expansion process. This work was supported by Russian Science Foundation, grant No. 24-19-00746.