Numerical simulation of the Rayleigh-Taylor instability in rarefied Ar/He mixture using the Direct Simulation Monte Carlo method

A V Kashkovsky, A N Kudryavtsev and A A Shershnev
Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, 630090, Novosibirsk, Russia
E-mail: sasa@itam.nsc.ru

Abstract. The Direct Simulation Monte Carlo method is used to study the emergence and development of the Rayleigh-Taylor instability. At the initial time, the heavier gas (argon) was located above the lighter gas (helium). In the simulation, no initial perturbations were superimposed on the interface, the appearance of instability was caused by fluctuations of gas-dynamic parameters that are inherent in the Direct Simulation Monte Carlo calculations. The onset of large-scale movement and mixing processes are investigated. Quantitative characteristics of the evolution of the Rayleigh-Taylor instability in a rarefied mode are obtained.

1. Introduction

Hydrodynamic instabilities emerge usually in the flows with sufficiently large Reynolds numbers occurring in the fully continuum regime. However, in a number of cases, particularly those associated with the action of bulk forces, instability can also manifest itself in the conditions where the continuum description is not fully applicable, and rarefaction effects play a significant role. One example is the Rayleigh-Taylor (RT) instability arising in a gravitational force field, when a layer of heavier fluid is located above the layer of a lighter one. In the continuum regime the development of the RT instability has been intensively studied for many decades on the basis of the Navier-Stokes equations, starting with the classical works [1,2], see also [3]. A review of the most important works can be found in [4]. In recent years, the equations of multi-velocity multi-temperature gas dynamics [5, 6] have also been used to model the development of the RT instability.

Modeling of the emergence and development of the RT instability in rarefied gas flows requires the use of a molecular kinetic approach. Numerical simulation is virtually the only theoretical tool that can be employed for this kind of research. However, both the molecular dynamics method and the Direct Simulation Monte Carlo method, DSMC (the latter is considerably more efficient for gas flows) require a very large computational resources due to the significant difference in spatial and temporal scales of the molecular movement and scales on which hydrodynamic instabilities develop.

The situation changed with the development of powerful computers. In recent years, papers have appeared in which the unsteady development of two-dimensional and three-dimensional disturbances in the RT instability was simulated numerically using both molecular dynamics [7, 8] and the DSMC methods [9]. The problem statement in these papers was exactly the same as in continuum simulations. At the initial time moment, a sine-shaped distortion of the fluid interface is assumed, so the initial
stages of instability development occur in a single-mode regime. In this paper, we use a different approach: it is assumed that the development of instability will be triggered by statistical fluctuations, which are always present in the DSMC calculations. As it will be seen, the picture of the development of instability in this case turns out to be significantly different and closer to its development in natural conditions.

2. Problem statement and numerical techniques
The problem of a plain layer of argon over a layer of helium in a field of gravity is considered (Fig. 1). At the initial moment, the temperature of both gases is constant and equal to 300 K, the pressure and density distributions along the vertical coordinate correspond to barometric formulas. Thus, the initial state is the analytical solution of the Euler equations. The top and bottom boundaries of the domain are isothermal walls with diffuse reflection of molecules and temperature of 300 K. Periodic boundary conditions are used at the lateral boundaries. The interface between gases at the initial moment of time is parallel to the \( x \) axis. The size of the computational domain is 100×100 m, the mean free path in helium and argon at the interface is \( 2.8 \times 10^{-2} \) and \( 8.8 \times 10^{-3} \) m, and the densities are \( 10^{-5} \) and \( 10^{-6} \) kg/m³, respectively. The pressure at the dividing line is 0.62 Pa. In order to reduce the difference between the characteristic times of instability and the characteristic molecular times, the acceleration of gravity \( g \) is increased to 1000 m/s².

Figure 1. Problem statement and computational domain schematics (a), initial density distribution along the \( y \) axis (b).

Numerical simulation was carried out using the SMILE++ software package [10, 11] developed in the Laboratory of Computational Aerodynamics of the Khristianovich Institute of Theoretical and Applied Mechanics SB RAS. From 12 to 60 million model particles and 26 cores of the computational cluster were used in the calculations. The time step was equal to \( 4 \times 10^{-6} \) s, the flow macroparameters stored on a grid of 200 × 200 cells. In order to reduce statistical fluctuations, the values of macroparameters in each cell were averaged over 1000 timesteps. The period of averaging was much shorter than a typical dynamic time of the instability development. Each cell was divided into 4×4 so called collision cells, used in the DSMC approach to sample pairs of particles which can collide during time step. A total of 2 million timesteps were made in the computation. Thus, 2000 frames were obtained representing the flow evolution.

3. Discussion of results
In Fig. 2 the total density flowfields of the gas mixture are shown at different time moments. Soon after the start of calculation, typical disturbances in the form of "fingers" appear on the interface surface. Their characteristic scale is such that about 10 structures fit into the domain length. There is a large-scale flow in which a heavy gas sinks down, penetrating the light one and vice versa. At the disturbed interface, a secondary Kelvin-Helmholtz instability emerges, leading to the formation of
vortices. Over time, they merge into larger mushroom-like structures (see Fig. 2c and Fig. 2d). At a certain point, the downward jet of heavy gas reaches the lower boundary and is partially reflected from it. In the end, an intense mixing occurs throughout the computational domain (Fig. 2e). All inhomogeneities merge into one vortex, the size of which is comparable with the size of the computational domain. Under the action of viscosity, the movement intensity should slowly decrease and the flow should gradually come to a steady state (Fig. 2f). The resulting picture of the development of instability is generally consistent with what is observed in numerous experiments (see, e.g., [12]).

![Figure 2](image.png)

**Figure 2.** Total density flowfields captured at different time instants.

It is obvious that in the final steady state, complete mixing of gases will occur, and each component will have a corresponding barometric distribution. The evolution of the flow can be characterized by the distributions of gas-dynamic quantities averaged along the horizontal direction. Figure 3 shows the density distribution evolution over time. It is obvious that by time $t = 0.8$ ms the main dynamic processes have already ended, and the stage of barometric distributions formations has started.

During the instability development, the gravitational potential energy transforms into kinetic energy, and through viscous dissipation, it transforms into internal energy. The gas heats up, but ultimately, due to the heat loss through the top and bottom walls, a uniform temperature distribution should be resettled. The potential energy in the final, more stable state is noticeably lower than in the initial one. Aforementioned energy transformation processes are shown in Fig. 4, where the time evolution of the kinetic energy ($E_k = \int_0^H \int_0^L \rho u^2 dx dy$), potential energy ($E_p = \int_0^H \int_0^L \rho gy dx dy$),
internal (thermal) energy ($E_i = \int_0^H \int_0^L \rho c_v T \, dx \, dy$), and total energy $E_t = E_k + E_p + E_i$ are shown. Note that in the kinetic energy calculation, we use the velocities averaged over the cell. Due to the fact that the cells for which the averaging is carried out cannot be considered as containing large, macroscopic number of particles, the calculated averages include large fluctuations. As a result, for example, $E_k$ is not equal to zero at the initial time.

It can be seen that the process of convergence to a steady state, in which the main role is played by viscous dissipation starts approximately from time $t \approx 1.5 \, \text{ms}$. The potential and internal energies oscillate in antiphases, and the amplitude of oscillation decreases with time. The cause of these oscillations is the compression and expansion of the gas in the lower part of the region. As for the total energy, it is virtually constant during the initial phase of instability development. However, further as viscous dissipation plays an increasing role, it starts to decrease, as the heated gas releases heat through the upper and lower walls. Obviously, in the steady state, the temperature throughout the region will return to the value of 300 K, and all the released potential energy will be removed from the system due to heat transfer.

To consider the change in the characteristic scales of the flow in the flow evolution process, the Fourier transform of the vertical velocity was performed along the original interface line ($y = 50 \, \text{m}$) and the corresponding spectra were extracted for different times (see Fig. 5). Since the spectral powers differ by several orders of magnitude for different points in time, they were normalized to the corresponding maximum values. It can be seen that disturbances initially occur, consisting of harmonics with wavelengths that fit 4, 7, and 12 times in the computational domain. In the process of development, the characteristic motion scale gradually increases, becoming ultimately equal to the length of the region.
Conclusions

The performed computations have shown that the development of the Rayleigh-Taylor instability can be successfully simulated at the molecular-kinetic level using the DSMC method. Moreover, in this case, there is no need to superpose initial perturbations onto the interface surface. The instability develops directly from the statistical fluctuations present in the DSMC method. Numerical simulation reproduces a physically realistic scenario of instability development with the emergence of finger-like structures, their growth, development into the vortical structures and mixing process.

The flow characteristics of mean and unsteady motion obtained from these computations seem to be similar to those observed in natural phenomena and physical experiments. The high level of statistical fluctuations, present in the DSMC method due to the substitution of real molecules by a much smaller number of model particles, does not change the general picture of development of the RT instability.

Acknowledgements

The current study was supported by Russian Science Foundation Grant No. 18-11-00246. This support is gratefully acknowledged.

Computational resources were kindly provided by Siberian Supercomputer Center of the Institute of Computational Mathematics and Mathematical Geophysics SB RAS (sscc.ru), Computational Center of Novosibirsk State University (nusc.nsu.ru) and Moscow State University Supercomputing Center (parallel.ru).

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