Simulation of an Evaporation of a Monatomic Condensed Phase into a Vacuum by a Monte Carlo Method

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Abstract. This paper deals with the study of the Knudsen layer value by Monte Carlo method. An escape of two particles from the monatomic condensed phase into the vacuum and a possibility of their collision were considering. The distribution of particle collisions in space and time were defined. These distributions for three-dimensional evaporations were determined. Computer experiments on the influence of temperature of the condensed phase and time delay of escape of the second particle dt on distributions were made.

INTRODUCTION

An investigation of a Knudsen layer structure is a main task for a conception of a mechanism of gas-surface interaction. In this layer take place considerable changes of gas flow values. It value is equal to a mean free path in gas phase. Certain interests present a question about formation of the Knudsen layer by the evaporation of the condensed phase. It is suppose that in this layer there are a little collisions. On the other side, if there are a mean values than must be a distribution of these values in space or time.

In papers [1,2] was get a distribution functions of a monatomic particles by speeds and energies after flight from the surface of the monatomic condensed phase into the vacuum by a Monte Carlo method. It was get results, which explained all physical phenomenons by the evaporation. In paper [3] was led investigation by a determine of the distribution of particle collisions in space and time by the evaporation of the monatomic condensed phase in case of two particles simultaneous flight from the surface.

This paper deals with the study of the flight of two particles from the monatomic condensed phase into a vacuum and a possibility of their collision by the Monte Carlo method. In every computer experiment 1000000 collisions were playing. The condensed phase has sizes 30Å x 30Å. Particles were a rigid sphere of a 3Å diameter. Computer experiments were made for a temperature region T from 1K until 1000K and intervals of particles flights dt from 10^{-13} s until 10^{-7} s. Positions of particles on the surface were played with a uniformly distributed generator of a random variables. Speed components of particles with a normally distributed generator of random variables were playing. By the flight of the first particle, the second particle is on the place during dt time and then it may fly out from the surface. It is necessary to note that the first particle may collide with the second particle until that moment when the second is on the place that is for time less than dt. This fact explains any especially of getting curves. The first collisions between two particles are playing the great role. They part is a main in compare with further collisions of particles.

RESULTS OF CALCULATIONS

Fig. 1 shows the data of calculation results of an average time of first particle flight t1 until of collision with the second particle. Present curves may explain the fact that in the region of low temperatures particles moves very slowly with comparison large temperatures.

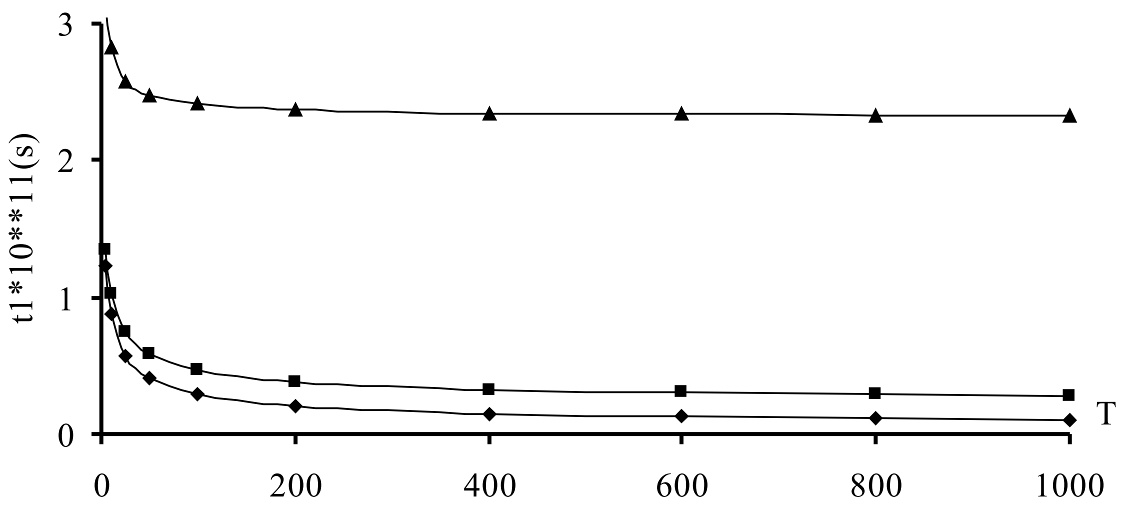

FIGURE 1. The average time distributions of first particle flight. ▲ – dt = 10^{-10} s, ■ - dt = 10^{-11} s, ♦ - dt = 10^{-12} s.

In Fig. 2 shows the density distributions of the first particles time motion t1 as a function of the condensed phase temperature. It is necessary to mark a presence of maximums, which coincides with dt = 10^{-13} s.

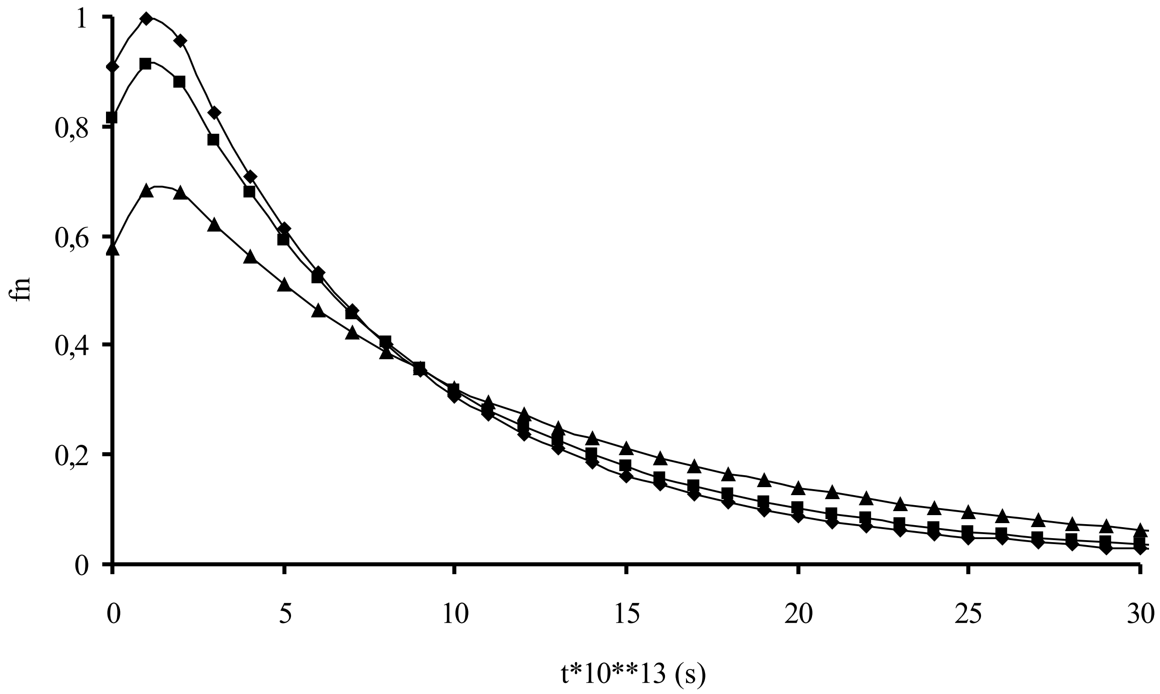

FIGURE 2. The density distributions of the first particles time motion. dt = 10^{-13} s.
♦ - T = 1000K, ■ – T = 800K, ▲ – T = 400K.

In Fig. 3 shows the density distributions of the first particles time motion t1 as a function of the dt values for the temperature T = 1000 K. For low dt there are the first maximums which coincide with the corresponding dt. The presence of the first maximum may explain as a collision of the first particles with the second particles when they were found at the condensed phase. Analogous distributions were getting for the other temperatures.

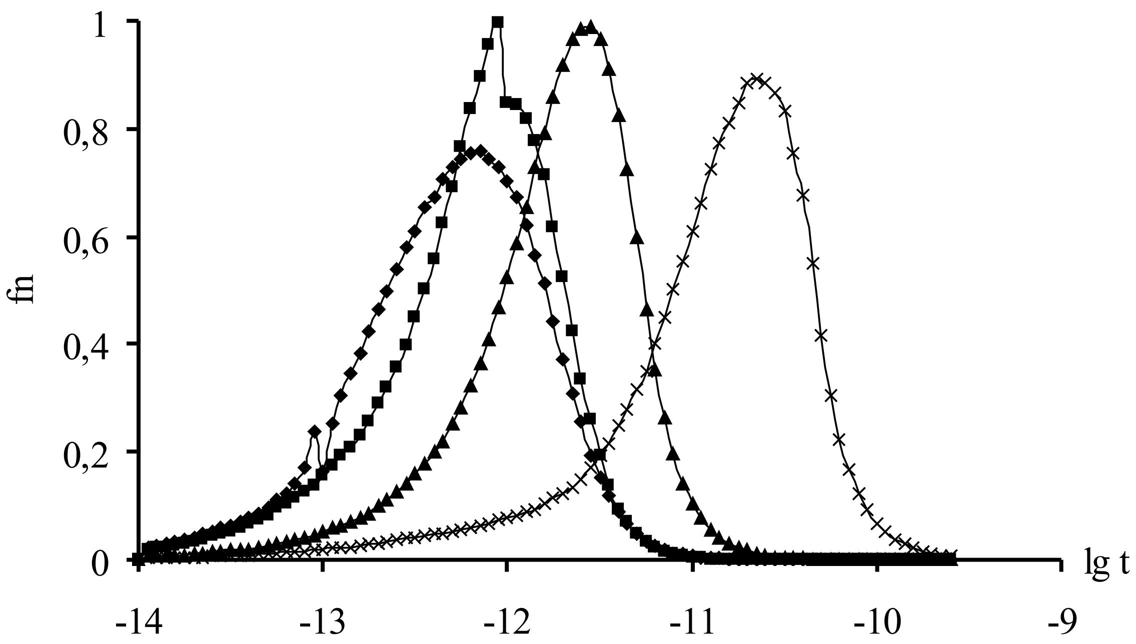

FIGURE 3. The density distributions of the first particles time motion.
T = 1000K. ♦ - dt = 10^{-13} s, ■ – dt = 10^{-12} s, ▲ – dt = 10^{-11} s, x - dt = 10^{-10} s.

The results of the calculations for the average values of distances in z - direction were showed on Fig. 4 for other temperatures and dt. For the low dt do not changes the average values. It may be explain that fact that the second particles do not fly out from the condensed phase still. For the large dt defining will be the particle collisions in the vacuum. For the more larges dt were get the analogous curves. If dt increase at 10 times then the corresponding values of z will be increase at 10 times too.

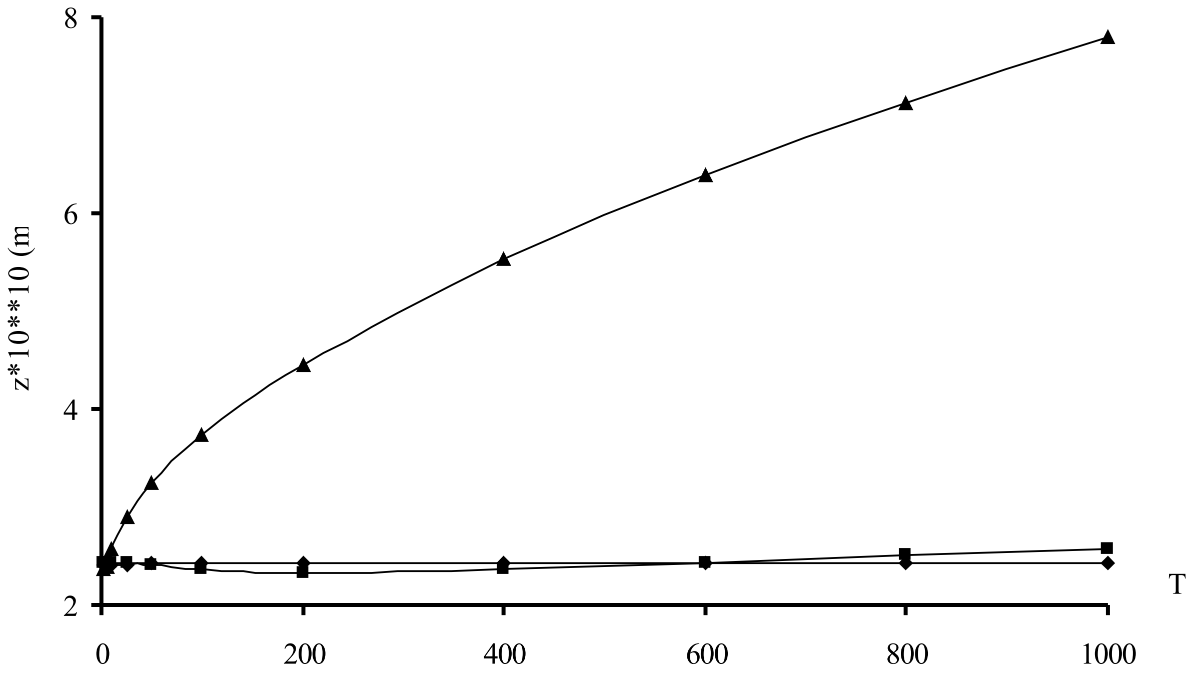

FIGURE 4. The average distance values z of the first particle collisions under the condensed phase.
♦ - dt = 10^{-13} s, ■ – dt = 10^{-12} s, ▲ – dt = 10^{-11} s.

In Fig. 5 the density distance distributions z of space collisions for T = 1000K are given. For the low dt the distributions have one maximum. For the large dt may see more complex structure of the distributions. For the large dt there are two clear maximums. The first maximum determined as the collision of first particles with second particles when they are in the condensed phase. The second maximum determined as the collision of first particles with second particles when they are in the vacuum.

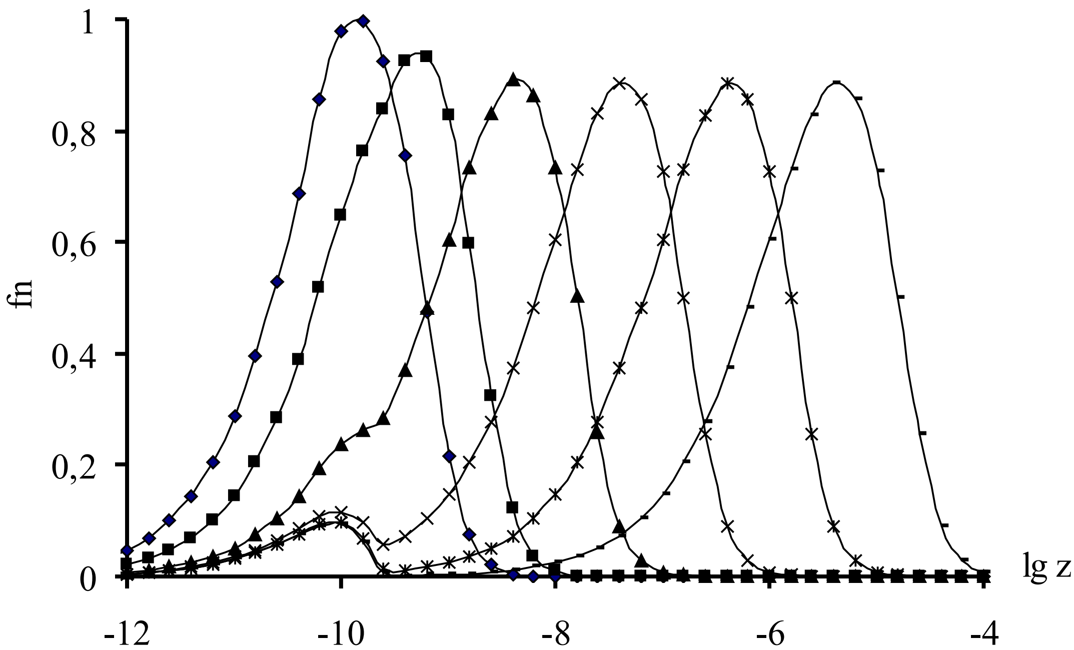

FIGURE 5. The density distributions of space collisions. T = 1000K.
♦ - dt = 10^{-12} s, ■ – dt = 10^{-11} s, ▲ – dt = 10^{-10} s, x - dt = 10^{-9} s, * – dt = 10^{-8} s, - – dt = 10^{-7} s.

One of the values, which were determine in computer experiments were a distance between of the particle centers a12. This value a12 may change from 6Å until 42,4Å. In Fig. 6 the average distributions of value a12 for other temperatures are presented. It is necessary to mark that the distributions of value a12 are qualitative difference for other dt.

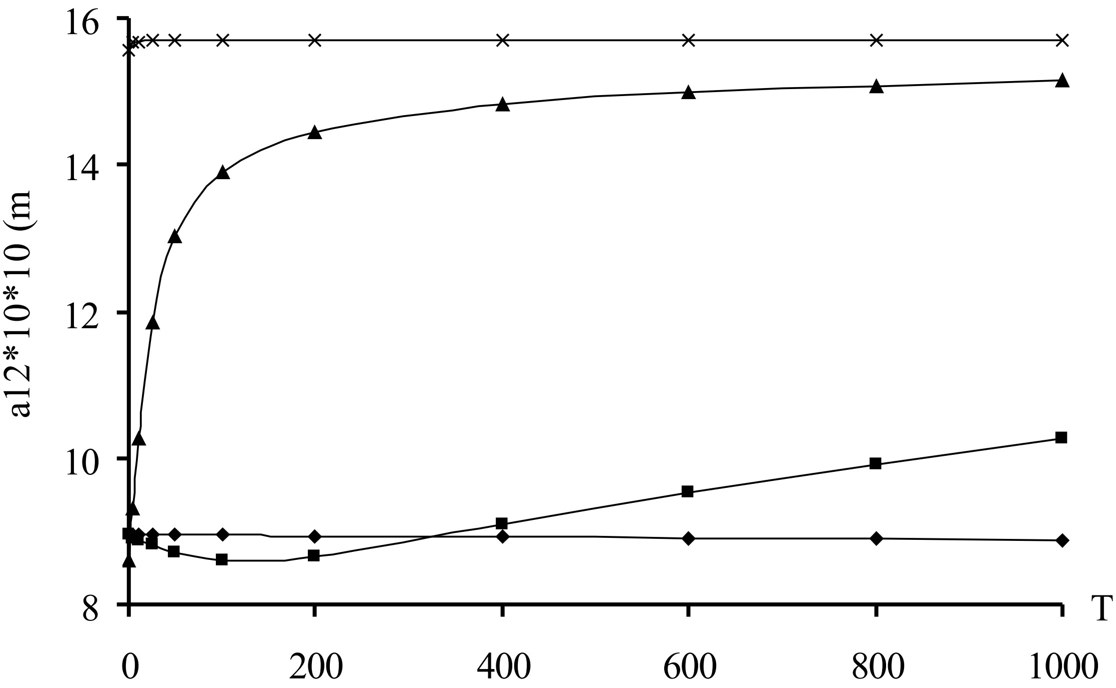

FIGURE 6. The average distributions of value a12.
♦ - dt = 10^{-13} s, ■ – dt = 10^{-12} s, ▲ – dt = 10^{-11} s, x - dt = 10^{-9} s.

In Fig. 7 the density distributions for the value a12 for the temperature T = 1000K for other values dt are given. There are two maximums on all curves. The first may clear see for the value dt = 10^{-13} s. The first maximum determined as the collision of first particles with the second particles when they are in the condensed phase.

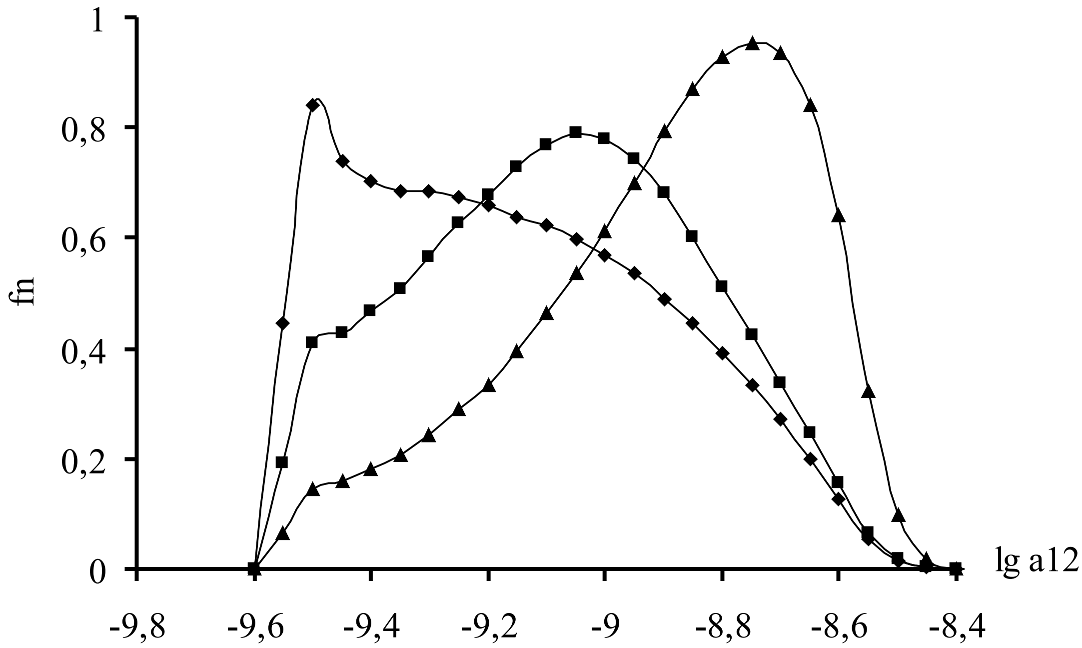

FIGURE 7. The density distributions for the value a12. T = 1000K.
♦ - dt = 10^{-13} s, ■ – dt = 10^{-12} s, ▲ – dt = 10^{-11} s.

CONCLUSIONS

The analysis of calculation results has showed that it is necessary take into consideration the collisions of fly out particles with the particles in the condensed phase. Because first particles may collision with second particles both in vacuum and in the condensed phase than it can influence on the processes of cluster formation and on the diffusion of particles on the surface of the condensed phase. An importance of such collisions will increase with increasing of a density of flying out particles flow. Such collisions will be playing the greater part by the computer modeling of fly out three, four, etc. number particles and by the molecular modeling method.

REFERENCES

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