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COMPUTER SIMULATION OF THERMODYNAMIC PROCESSES FOR EDUCATIONAL PURPOSES

The paper describes simulation model of the ideal gas, constructed according to the laws of mechanics, applied to numerous simple objects. Objects of the study are perfectly elastic balls, having certain mass and size. Balls collide with each other and with the walls of the vessel elastically, i. e., without energy losses for plastic deformation. Calculation of the collisions follows from the laws of conservation of energy and momentum, this is necessary condition of model physicality.

Balls move in the discrete time, i. e., their coordinates and pulses change by jumps, that is actually numerical solution of differential equations of motion. Relation between the discrete time and real is determined by the frequency of the program mover and is within 10 to 100 cycles per second. Frequency of mover operation depends on the power of the processor and on the complexity of the investigated model. Gas model is 2D, this reduces the number of the necessary calculations to the acceptable value and enables to use model for creation of the interactive study guide.

On the base of the model the computer program is developed, it enables to simulate the laboratory installations and carry out the experiments. Installations consist of vessels, vessels with the pistons, heating and measuring devices. Experiments may cover wide spectrum of the phenomena, such as diffusion, Brownian motion, various kinds of heat capacity of gas, division of particles velocity, conversion of the thermal energy into mechanical, different thermodynamic cycles, etc.

Although computer simulation is not viable substitute of physical experiments, it is flexible and able to reproduce far more experiments than any school or institute laboratory. Computer model promotes the development of the experimental skills of the students and makes educational process more interesting and efficient.

Key words: *ideal gas, simulation model, computer simulation, educational process.*

Introduction

Classic thermodynamics is an important branch of physics, which is not simple for comprehension. Difficulties are connected with the lack of physical intuition regarding gas behavior and such notions as enthalpy, entropy, isochoric and isobaric heat capacity. Such situation could be improved if the study of the theory is supported with sufficient laboratory practice, but for known reasons now it is impossible. However, with the development of hardware and software of the computers wide possibilities open for the software simulation of physical phenomena even using notebooks and smartphones. It is important to note, that such simulation does not violate the laws of physics and is of interactive character because only active actions of the learner provide the successful study.

In the given study simulation model of ideal gas, constructed on the base of the laws of mechanics, applied to large number of simple objects is suggested. Idea of simulation of gas behavior by means of numerous objects is not new [1]. Studies in this field are devoted to achieving external similarity with the reality [2, 3] or improvement of the accuracy of separate phenomena simulation [4, 5, 6], for instance, taking into account Lennard-Johnson potential [7] during particles collision.

The problem with the computer simulation is that there must be sufficient amount of particles (tens or even hundreds of thousands), to produce statistic character of gas behavior. At the same time computations must be carried out rather rapidly to conduct the «laboratory investigations» in real time. Additional requirement is that the model should operate in wide range of the values of its parameters because this makes the investigations more varied and more meaningful.

Model

For modeling the ideal gas «billiard balls» - absolutely elastic spheres, having certain mass and size are used. Balls collide with each other and with the walls of the vessel elastically, i. e., without loses of energy for plastic deformation. Calculation of the collisions proceeds from in laws of conservation of energy and momentum, this is important, although non sufficient condition of physical model.

Balls (further they will be called particles) move in discrete time. Ratio between the discrete time and real is determined by the frequency of the programming mover operation and is within the limits of 10 to 100 cycles per second. Frequency of the mover operation depends both on the power of the processor and complexity of the investigated model.

Gas model is two-dimensional, this reduces the complexity of creating the «laboratory installations» by the user to acceptable level. Also this greatly reduces the amount of calculations, needed for gas behavior simulation.

Summing up the above-mentioned, the following factors of risk of the model inadequacy can be mentioned: discreetness of time, relatively small number of particles and two dimensionality of the modeling space.

Reflection of the particles from the walls of the vessels

In the first versions the models of the vessel with gas were polyhedrons of an arbitrary form. But later it turned out that this form was not very useful and now the form of the vessel is limited by the polygons, where all the angles are right and the edges are parallel to the coordinate axes, as a rule, these are rectangles. Restrictions imposed do not decrease the teaching value of the model but simplify computations, this, in its turn, enables to increase the amount of particles and approach the model to reality.

Particles move inside the vessel, reflecting from the walls. The size of the particles while calculating their collusions with the walls will be neglected, this corresponds to the concept of ideal gas and simplifies calculations.

Let x_t, y_t – be the coordinates of the particle at the moment of time t, and vx_t, vy_t – is the speed of the particle at this moment. Wall of the vessel is the section of the direct line, the ends of this section have the coordinates x_1, y_1 and x_2, y_2. If there are no obstacles at the next moment of the discrete time the coordinates of the particle will be:

$$x_{t+1} = x_t + vx_t \text{ , } y_{t+1} = y_t + vy_t \quad (1)$$

In the formulas (1) the interval of the discrete time between the moments t and t+1 equals one, that is why, multiplication of the speed by one is omitted.

It is believed that at the moment of time t particle collides with the wall, if sections $((x_1, y_1), (x_2, y_2))$ i $((x_t, y_t), (x_{t+1}, y_{t+1}))$ are intersected. In case of the absolute elastic collision of the particle with the wall the component of the particle speed, directed along the wall, does not change and the component of speed, normal to the wall, changes its sign into opposite (Fig. 1 a).

It may happen that the particle, reflected in such a manner will be outside the limits of the vessel (Fig. 1 b). To prevent this from happening it is necessary to take into account not one but all the collisions of the particle with the walls, which might happen if the particle were real. The higher is the speed of the particle, the more collisions take place (Fig. 1 c).

Mutual collisions of the particles

Some models of the ideal gas do not take into account the collision of particles at all [8]. But in our case it is not acceptable because in this case we do not have a possibility of modeling many phenomena such as diffusion, distribution of particles speed, balancing of the particles system, etc.

In the current version of the model the collision of two particles is considered to have happened, when the distance between their centers, first, becomes smaller than the sum of their radii, second, will decrease, if the motion of the particles continues (Fig. 2a).

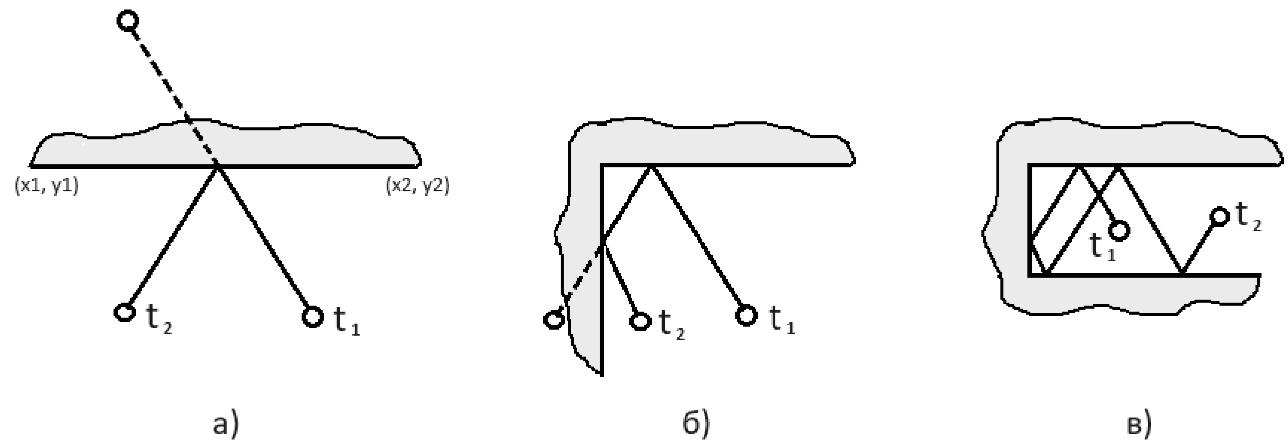

Fig. 1. Reflection of particles from the walls of the vessel

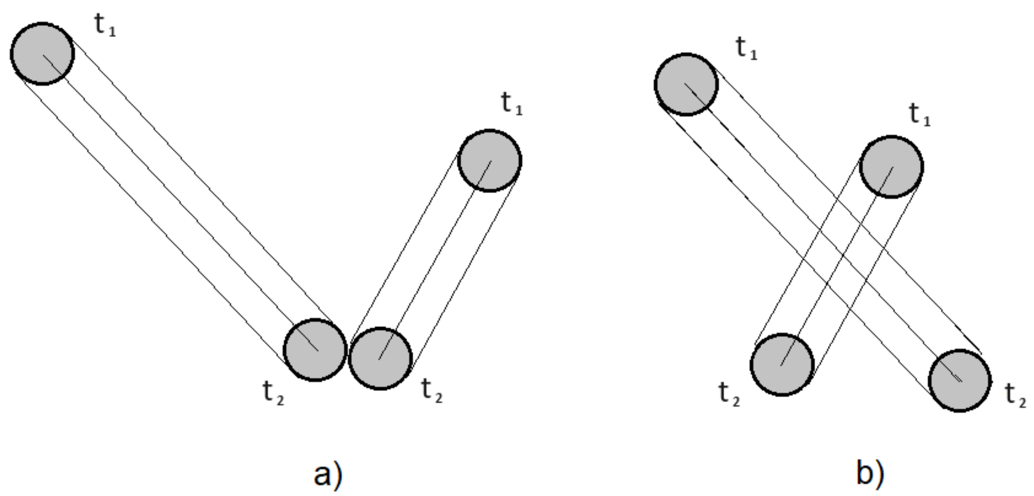

Fig. 2. Collision of the particles

Possibility of simultaneous collision of three and more particles in the model is not considered.

Collision occurs absolutely elastically that is why, the calculation is performed according to the laws of conservation of total energy and momentum of two particles [9].

Calculation starts from the turn of the calculation system so that the line, connecting the centers of balls be parallel to Ox axis. In such position of the balls in the case of collision only the projections of speeds on the axis Ox change, and projections of speeds on the axis Oy remain unchanged.

If m1 and m2 – are the masses of balls prior to the collision, v1 i v2 – speed of balls after collision, u1 and u2 – are speeds of the balls after collision, projections of the speeds on the axis Ox are determined by the formulas:

$$u1_x = \frac{((m1-m2)*v1_x+2*m2*v2_x)}{m1+m2} \tag{2}$$

$$u2_x = \frac{((m2-m1)*v2_x+2*m1*v1_x)}{m1+m2} \tag{3}$$

Calculation is completed by the rotation of the calculation system in the reverse direction.

If the collision conditions are verified only in discrete moment of time (as it is done now), the collisions, which would have taken place, if the time of the model was continuous but not discrete, will not be noticed (Fig. 2b). It is possible to take into account such collisions but it is not expedient as the volume of computations in this case drastically increases. At the same time it is clear that the role of collisions of the particles between themselves is reduced to redistribution of the particles speeds (or their kinetic energy) within the limits of the space, occupied by particles. The more collusions, the more rapid is the redistribution and the system more rapidly passes in the balanced state.

If the accounted collisions are few, transient processes in the model slow down and its monitoring is not comfortable. Increasing the radius of the balls the number of collisions will be brought to the acceptable level. The acceptable number of collisions will be discussed, when the limits of model application are determined.

If the possibility of the collision\ for each pair of particles in the model space is verified, the number of needed verifications will be assessed as $O(n^2)$, where n – is the amount of particles. Such conclusion follows from the fact that the number of pairs, created from the elements, equals $n(n-1)/2$.

However, the collisions are more probable with the nearest neighbors of the particle and is improbable with remote particles. Modal space can be divided into cells and verification of the possible collisions can be carried out within the limit of the cell, where the particle is located. At each cycle of modeling time distribution of particles by the cells must be updated.

Division of the space for the cells will lead to further loss of the potential collusions, because possible collisions between particles, close to each other but are located in different cells will not be taken into account. But, as it was already mentioned, account of all collisions is not obligatory and it can be neglected for the sake of efficiency. Although the division of the space into cells does not change the assessment of $O(n^2)$ time complexity of calculations, it can decrease their number by two orders.

However, as the experience showed, stable borders between cells and fixed order of their bypass lead to non-desirable effects in gas behavior, which become noticeable at low temperatures, i. e., at very low speeds of the particles. It should be noted, that such phenomena were eliminated by means of changing the order of cells bypassing on the opposite at each cycle of the discrete time.

Measurement

To following the processes taking place in the model, the measurements of temperature and pressure in the preset volume of gas are needed. Taking into account the mechanical nature of the model such things as total number of particles, volume, they are located, mass and speed of each particle can be observed. Indices of the pressure and temperature will be derivatives from the above listed.

Determination of the temperature:

$$T = \frac{2}{i}\frac{\varepsilon_{aver}}{k_B}, \tag{4}$$

where T – is the gas temperature, $\varepsilon_{\text{aver}}$ – is average kinetic energy of particles, i – is number of freedom degrees (for 2D model it equals two), k_B – is Boltzman constant.

Average kinetic energy is calculated as $\varepsilon_{\text{aver}} = \frac{\varepsilon_{\text{tot}}}{N}$, where N – is the amount of particles in the area of measurement, ε_{tot} – is total kinetic energy of all the particles. Thus, for temperature measurement it is sufficient to know the total kinetic energy and the amount of particles in the area of measurement.

$$T = \frac{\varepsilon_{tot}}{Nk_B} \tag{5}$$

From basic gas equation

$$pV = Nk_BT \tag{6}$$

it follows that the pressure is the relation of the total kinetic energy of the particles to the volume they occupy.

$$p = \frac{Nk_BT}{V} = \frac{\varepsilon_{tot}}{V} \tag{7}$$

That is, pressure as temperature, depends in the model only on the total energy and amount of particles in the measured volume, for the determination of the pressure it is sufficient to know the total energy of particles and the volume of the measurement area.

In case of such measurement Charles law (p/T= const if V=const)

$$\frac{p}{T} = \frac{\varepsilon_{tot} / V}{\varepsilon_{tot} / Nk_B} = \frac{Nk_B}{V} \tag{8}$$

and Boyle-Mariottes law (pV = const if T=const)

$$pV = \frac{\varepsilon_{tot}}{V} V = \varepsilon_{tot} \tag{9}$$

are executed automatically. But practical verification of both laws is expedient because it is verification of the computational correctness of the model.

Verification of the ratio pV= const can be performed by means of the installation, which is a vessel, containing 3 parts or sections in the relation 1:2:4 (Fig. 3a).

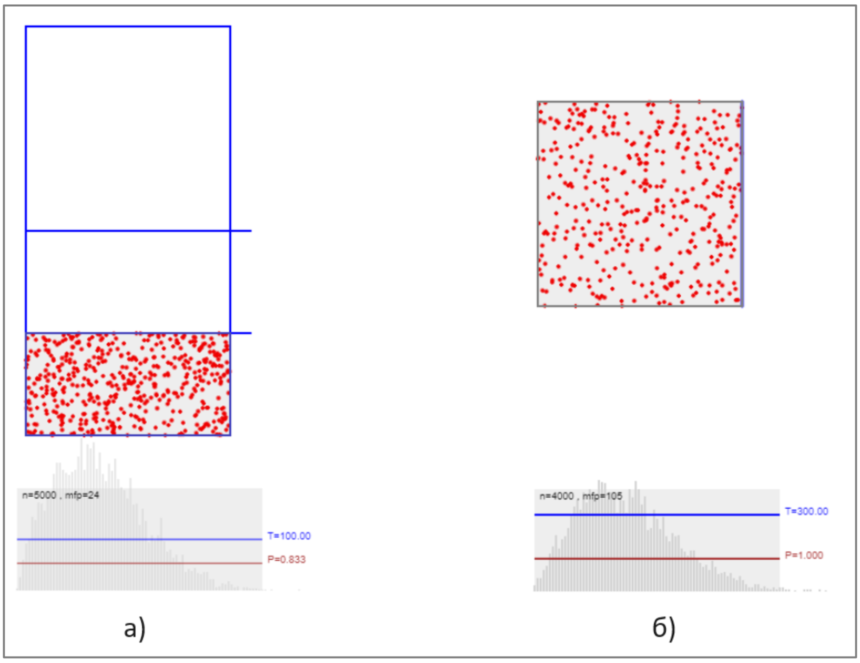

Fig. 3. Verification of Charles and Boyle-Mariottes laws

In the lower section of the vessel there is certain volume of gas, its pressure and temperature are measured by means of certain device. The device calculates energy and number of particles within the limits of the rectangular of the device (in the figure the rectangle is colored in grey). Contour of the device rectangle is also grey and coincides with the boundaries of the section, that is why, it is not well seen. Device readings in digital and graphic forms can be seen below the image of the vessel, more information about the devices will be presented further.

Low valve will be removed and the gas will occupy two times larger volume and the pressure is measured again. It is known that when the gas expands in vacuum its temperature does not change, because it does not perform work, but the temperature is also measured directly.

The second valve will be removed, this will increase four times the volume of gas, then the pressure will be measured again. The parameters of the installation are the following: total volume of the vessel V = 200*400, amount of gas particles N = 5000, temperature T = 100, radius of the particle r = 0.25, mass of the particle m = 1. The results of pressure measurements are shown in Table 1.

Table 1.

Boyle-Mariottes Law

V	p	pV
200*100	0.833	16660
200*200	0.417	16680
200*400	0.208	16640

Verification of p / T = const relation will be made for the vessel with gas, which will be heated and cooled by means of heating device, simultaneously pressure will be measured (Fig. 3b). The parameters of the installation are the following: total volume of the vessel V = 200*200, amount of gas particles N = 4000, radius of the particle r = 0.25, mass of the particle m = 1. Results of temperature and pressure measurements are shown in Table 2.

Table 2

Charles Law

T	P	p / T
199.30	0.664	0.003332
300.00	1.000	0.003333
399.32	1.331	0.003333

Measuring devices

Measurements are performed in the rectangular area of the space, by means of program objects – measuring instruments. During one cycle of the model time measuring instrument counts the number of gas particles, locating within the limits of the rectangle of the instrument, their total and average kinetic energy. Results of measurements are presented in the form of temperature and pressure values.

Devices can be created when they are needed and eliminate when the need for them disappears. The device can be tuned for measuring partial pressure and temperature, selection is performed by the color of particles.

On the screen the device looks like semitransparent rectangle of grey color. Readings of the device are indicated on a separate panel near the rectangle of the device. Values of pressure and temperature can be seen there in digital and graphic form. Last 50 measurements participate in the construction of graphs, this enables to monitor not only the instantaneous values but also the trend of their change.

Measuring device also displays histogram of molecules speed modules. By the type of such distribution it can be assessed if the gas is in the balanced state – when the system of particles is in the balanced state, distribution must approach to Maxwell-Boltzman distribution [9].

Fig. 3 shows how measuring instruments, and their readings look like.

Heating devices

Heating device either supplies or takes away heat from the gas. The parameters of the device: rectangle in space (set by the coordinates of the left upper x1, y1, and right low x2, y2, angles) and rate – heating speed. Device acts on the gas, located in the rectangle.

At each cycle of the discrete time the device increases the speed of each particle by the formula v = v * rate. If rate> 1 the device transfers heat to gas, if rate < 1, vice versa, takes away. The device counts the total amount of the transferred heat, it is positive during heating and negative during gas cooling.

The device looks like semitransparent rectangle of the orange color when it heats the gas and blue color, when it cools the gas. As measuring instruments, heating devices are created and eliminated if necessary.

Measuring units

Values of the models parameters (pressure, volume, temperature etc.) can be expressed in conventional units and this will not have any impact on the results of research, initiated on the model. Conventional (or model) units are chosen to decrease the number of coefficients in the formulas, according to which calculations, necessary for model functioning, are made.

For the sake of convenience for the observers model units of measurement can be replaced during measurements results display by more habitual – centimeters, degrees, atmosphere, etc. Basic units can be renamed, model unit of the length can be named centimeter, unit of mass – gram, unit of time – second. Derived units – pulse, force, energy, pressure will be expressed by means of basic units.

Regarding the degrees, the range of possible speeds of particles should be taken in consideration. The scene will be created, where in the vessel of the volume 200x200 there are 4000 particles, mass of each is 1 and radius is 0.25. If the particles move at average speed 0.1, i. e., 1 pixel per 10 cycles of model time (approximately 5 pixels per sec), this looks very slow, almost of the boundary of acceptable for perception. Let us assume, that this corresponds to the absolute temperature of 1 degree.

By determination $T = \frac{\varepsilon_{\text{aver}}}{k_B}$ «Boltzmann constant» will be calculated for our model, k_B = 0.005. Now we have the coefficient of conversion of kinetic energy of the particle into absolute temperature.

It is known that in real life normal conditions correspond to 300 degrees and 1 atmosphere. But in model units the pressure in such configuration will become $p = \frac{\varepsilon_{\text{tot}}}{V} = \frac{N\varepsilon_{\text{aver}}}{V} = \frac{NTk_B}{V} = 0.15$. It follows, that at reflection of pressure measurements we must divide them by 0.15.

Relation between model and usual units of measurement can be presented in Table 3.

Table 3

Model and physical units of measurement

Value	Model unit	СГС unit	СГС / model
Length	pixel (p)	cm	1 / 1
Time	cycle (t)	s	1 / 50
Mass	unit of mass (m)	g	1 / 1
Force	$m*p/t^2$	$g\cdot cm/s^2$	2500 / 1
Energy	$m*p^2/t^2$	$g\cdot cm^2/s^2$	2500 / 1
Pressure	unit of pressure (m/t^2)	atm	1 / 0.15
Temperature	degree	degree	1 / 1

Pistons

Movable walls of the vessels are called pistons. Pistons are mainly used for modeling the conversion of thermal energy into mechanical and vice versa. Due to the pistons the cycles of thermal and cooling machines, both rotating and nonrotating can be reproduced. When pistons are used, moving wall of the rectangular vessel is located between two vertical walls and moves in vertical direction (Fig. 4a).

External force may act on the piston, it is directed from top to bottom. For the observer it looks like loading on the piston, exercised by a certain mass in constant gravitational field. External force is balanced under the pressure of gas under the piston or is not balanced and in this case the piston moves.

Piston motion is exclusively the consequence of gas particles hits and gravitational force, acting on its load. Gas particles, colliding with the piston, transfer it the pulse, as a result, at each moment of model time the piston moves at certain distance.

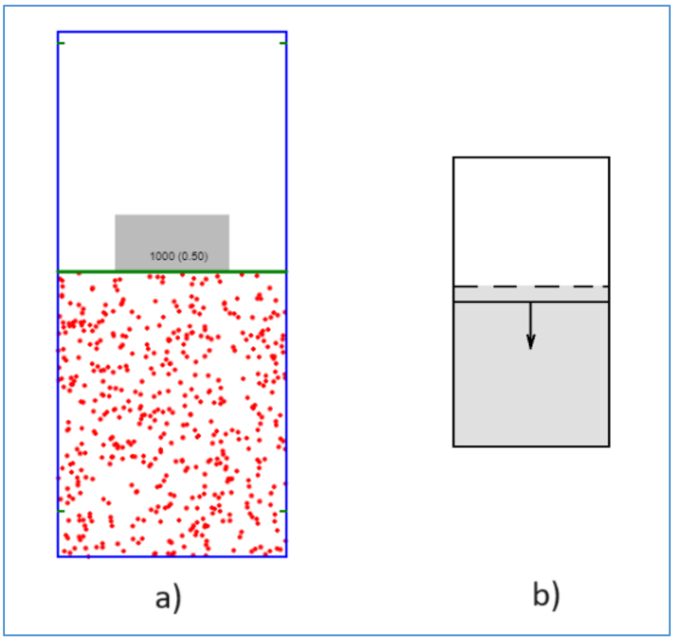

Fig. 4. Vessel with piston

Piston shift occurs when all the gas particles obtained their new location and if in the space, traveled by the piston, there are particles, they will be outside the piston (Fig. 4b). To avoid this, such particles are shifted vertically on the length of the piston route. This does not influence the model behavior, as the speed of particles does not change and the size of the shift is insignificant.

As such model does not provide energy dissipation, any deviations from the balanced state, such as heating or cooling of the part of gas, motion of the piston, etc, provide the balancing process oscillating character. To avoid excessive oscillations of the piston, motion speed of the piston can be limited. Such limitation results in energy loss and can be cancelled, if such oscillations do not hinder the course of research.

Measurements, performed by measuring instruments are also connected with the pistons, measuring rectangle is considered to be part of the vessel under the piston. Besides the pressure and temperature, the work, performed by the gas against gravitation force and energy losses as a result of speed limitation, if it is the case , is taken into account.

Limits of model application

Spheres of model application are such combinations of its parameters at which basic gas law is realized. For instance, measured gas pressure under the piston must be equal to the pressure, created by the external force, in case, when the piston does not move, or actual distribution of particles speed in the balanced system must approach Maxwell-Boltzmann distribution.

Sphere of application can be described as a part of the model parameter space, where the model behaves correctly. It is difficult to outline correctly this part, because the model parameters besides pressure, volume, temperature comprise the size of particles, their mass and total amount. That is why, it would be convenient to use one of these index, which would prove that the model is within the admissible limits and measurement data can be relied upon.

This index should be the measure of the model approach to the ideal gas and this may be average length of the free path of the particles, relative space of which is occupied by the particles in the vessel, ratio of the particles collision per unit of time to their amount, etc. Let us stop at the average length of free path, as at the most frequently used. Average length of free path can be assessed if the total path, covered by the particles during one cycle of model time is divided into double number of collisions between particles during the same time (one collision interrupts the paths of two particles).

Length of the route, covered by one particle during one cycle of model time can be measured directly on the base of the particle location in two adjacent moments of time. This is correct, because the collision of particles are recorded only at the end of their paths, all other possibilities of collision are ignored (Fig. 2).

Particles, experienced the collisions with the walls, are excluded from the count. This does not influence greatly the result, because it does not depend on the exact number of particles, participating in the calculation of the average value.

As a result of the experiments it was determined that the model behaves correctly if average length of the free path is not less than 50 – 100 model units of length. Two values are given because the boundary depends on the temperature of the gas, for low temperatures it is approximately 50, for high temperatures 100.

The essence of the experiments was that the vessel with piston was filled with the gas at certain temperature and load on the piston. Further the gas pressure under the piston was measured and compared with the pressure, created by the external load on the piston. If indices of external and internal pressure coincided, the behavior of the model was considered to be correct. In a series of measurements the gas temperature and loading on the piston remained constant, only the size of the particles changed.

Data of two series of measurements are given in Table 4. Zone of the parameters, where model behavior was correct, is colored in grey. General parameters of both series of measurements are the following: number of particles 5000, mass of a particle 1, volume of the vessel under the piston from 40000 to 70000 square units, depending on the position of the piston. Every measurement was carried out after balancing of the system, which took place during 1000 cycles of discrete time.

Table 4

Area of the model correctness

	T=100, P=0.25		T=1000, P=2.5	
Radius of the particle	Measured pressure	Average length of the path	Measured pressure	Average length of the path
0.0625	0.250	1050	2.50	5532
0.125	0.250	230	2.50	1011
0.25	0.250	58	2.50	260
0.5	0.245	15	2.49	65
1.0	0.223	4	2.45	17
2.0	0.137	1	2.30	5

Model behavior in the zone of incorrectness can be explained by the fact that when the density of the particles is great, their complete internal energy consists of kinetic energy of motion and potential repulsion energy due to mutual collisions of the particles. Pressure of the gas, balancing the external pressure on the piston, depends on the complete energy of the gas but only kinetic energy is measured. This is where the discrepancy arises, which is greater , the greater share of potential energy in the complete energy.

Software realization

Computer simulation is realized in the form of one-page web-application [10]. User is given laboratory setup designer and command panel. Fig. 5 shows window interface of the program. User can create its own setup or load one of the already prepared.

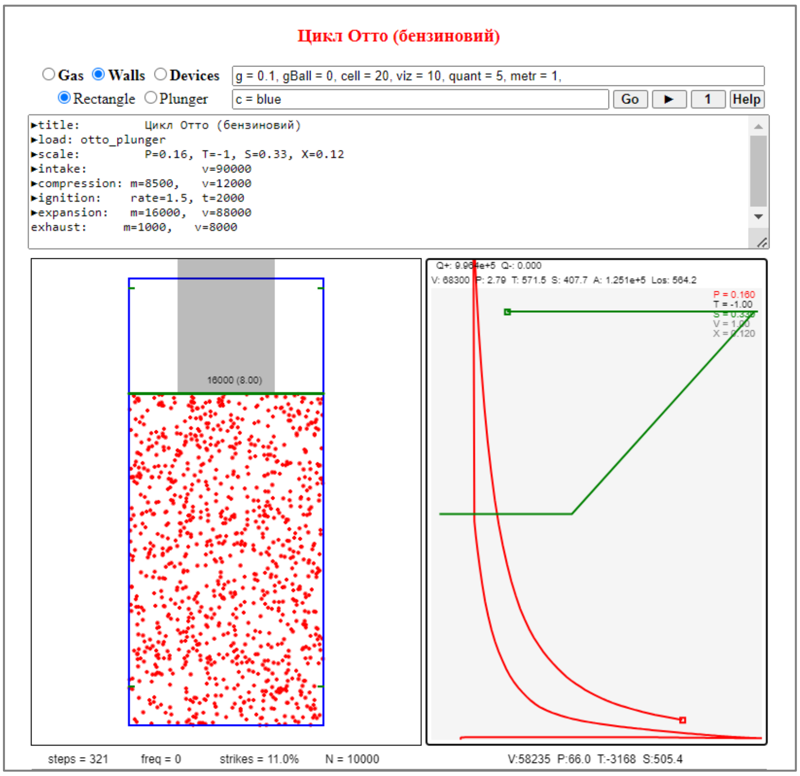

Fig. 5. Computer simulation of thermodynamic processes

Setup is formed by adding various objects. Designer of the setups operates in three modes: Gas, Walls and Devices. In each mode corresponding objects can be added. Properties of new object are set in the input field in the form of pair «key = value». Type of new object is chosen by radio buttons.

In the command panel the user adds one or several commands, they concern simulation of thermodynamic processes. Commands are executed by the interpreter and at the same time in the left part of the screen the behavior of the laboratory setup is demonstrated and in the right part numerical and graphic characteristics of the processes, taking place.

Conclusions

The paper suggests the computer model of ideal gas, it reproduces rather accurately gas behavior and can be used for the simulation of laboratory research in the process of studying physics and thermodynamics. The model was examined for the correctness, boundaries of its application were outlined.

On the base of the model the computer program was developed, it enabled to simulate the laboratory setups and carry out the experiments with their help. Experiments may comprise wide range of phenomena, such as diffusion, Brownian motion, various types of heat capacity of gas, distribution of particles speed, transformation of thermal energy into mechanical, different thermodynamic cycles, etc.

Although computer simulation is not a comprehensive replacement of real laboratory studies, it is flexible and can reproduce far more experiments than and school or university laboratory. Computer model promotes the development of research skills of students and allow them to make the way, similar to the way covered by the first inventors.

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