CALCULATION OF THE PARAMETERS OF CRYOGENIC VACUUM CHAMBERS BY THE MONTE CARLO METHOD

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The main parameters of cryogenic vacuum chambers are examined and the possibility of their calculation by the Monte Carlo method is shown. An algorithm for calculating the parameters and its realization on a computer are described.

Many authors [1–4] have used the Monte Carlo method and high-speed digital computers to calculate the parameters of various elements of cryogenic vacuum chambers. Mainly, the probabilities of certain events, such as, for example, a gas molecule hitting a cryogenic element, have been calculated.

This paper shows the possibility of calculating by the Monte Carlo method the main parameters of a chamber that directly characterize the vacuum when the local laws of behavior of molecules are known. These parameters include, for example, the molecular concentration in the chamber and the evacuation rate of the pumping system. It is shown how these parameters are simply expressed in terms of the mean lifetime $\bar{t}$ of a molecule in the chamber. If we simulate a random value t (the lifetime of molecules in the chamber) and determine its arithmetic mean in N tests, we can approximately determine $\bar{t}$ and the parameters that interest us. The parameters that have the meaning of the probabilities of certain events are described.

To make the method accessible for practical calculations, general-purpose programs were written for the M-20 computer. The programs are general purpose in that they need not be changed when calculating the parameters of a new chamber—only new input data must be given. This is achieved by a uniform method of tracking molecule trajectories, regardless of the specific nature and complexity of the chamber geometry.

Parameters of the Cryogenic Chambers. Cryogenic chambers are used to produce a high vacuum. The pump in such a chamber is represented by surfaces, cooled to the hydrogen or helium temperature, on which the gas condensation occurs.* Figure 1 shows a cross section of a cylindrical chamber. The shields are usually at the nitrogen temperature and are placed so that the thermal flux to the cryogenic elements does not exceed the critical value and so that the consumption of cryogenic fluids is reduced. In addition, certain gas components are condensed on the shields.

The main characteristic of a vacuum chamber is the number of gas molecules in the chamber in steady-state operation; we shall call this number N_c. The gas flow into the chamber is determined by the intensity of the source (inleakage), i.e., the number of molecules that enter the chamber in 1 sec, which we shall call q. The removal of particles from the chamber occurs when they are captured by the pump system, and is characterized by the discharge intensity r, i.e., the number of molecules evacuated per second.
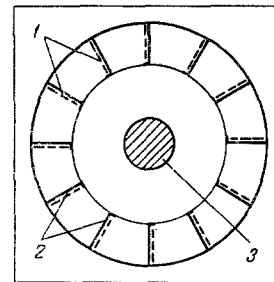

Fig. 1. Cross section of a chamber with a cryogenic pump: 1) cryogenic elements; 2) shields; 3) object.

Let the source intensity q be constant with time. We shall make the following assumption about the discharge intensity r: at any time it is proportional to the number of molecules in the chamber, i.e.,

$$r = \sigma \bar{N}, \tag{1}$$

where σ is the capacity of the pump system—its main characteristic.

Steady-state conditions mean that q = r. If we substitute for r its value (1) under steady-state conditions, we obtain $q = \sigma N_c$. Then,

$$\bar{N}_c = \frac{q}{\sigma}. \tag{2}$$

The mean concentration $\bar{n}_c$ of molecules in a chamber of volume V is defined in terms of the parameter σ as follows:

$$\bar{n}_c = \frac{\bar{N}_c}{V} = \frac{q}{\sigma V}. \tag{3}$$

The "pumping rate" parameter S is also easily defined in terms of σ:

$$S = \frac{q}{\bar{n}_c} = \sigma V. \tag{4}$$

Since the chamber volume V and the inleakage q are given, the problem of determining $\bar{N}_c$, $\bar{n}_c$, and S reduces to finding σ. To make it possible to calculate σ by the Monte Carlo method, let us explain the sta-

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*Other pumps, whose operation will not be considered here, are usually used along with cryogenic shields in the chamber.

tistical meaning of this parameter by examining the removal of molecules from a chamber.

A molecule escapes from the surface of the source and, having been reflected several times from the surfaces of the chamber, after a certain time t is absorbed by one of the cryogenic elements. This time interval—from the moment of escape of a molecule to its absorption—we shall call the lifetime of a molecule in the chamber. Let us introduce the mean lifetime $\bar{t}$ of a molecule in the chamber. Then, if the chamber contains $\bar{N}$ molecules, each of which lives, on the average, $\bar{t}$ seconds, the number of molecules that leave the chamber in 1 sec (the discharge intensity r) is given by the relation

$$r = \frac{1}{\bar{t}}\, \bar{N}. \tag{5}$$

Comparing expressions (1) and (5), we obtain

$$\sigma = \frac{1}{\bar{t}}. \tag{6}$$

A convenient parameter for evaluating pump design is the mean path $\bar{l}$ of a molecule before absorption, which is a function of the chamber geometry (its design characteristics) and of the quality of the cold shields. This parameter is related to $\bar{t}$ as

$$\bar{l} = \bar{v}\,\bar{t}, \tag{7}$$

where $\bar{v}$ is the mean velocity of a molecule in the chamber.

Thus, the parameter $\bar{l}$ contains essential information about the chamber design. Calculation of $\bar{l}$ by simulation is much simpler than that of $\bar{t}$, and it does not require knowledge of the local laws of variation of molecule velocity.

The molecular concentration at a point M can be determined as follows.* We isolate within the chamber a cube of unit volume ΔV whose center is at point M and record for each molecule its residence time in volume ΔV, which we call Δt. Then, using the mean time $\overline{\Delta t}$, the concentration is written as

$$n(M) = q\,\overline{\Delta t}. \tag{8}$$

Along with the parameters that characterize the vacuum in a chamber directly, in many cases it is useful to consider the parameters introduced in [1,5, 6], which characterize the absorptivity of a pump system. We shall describe the more common of them here.

The capture coefficient α of an individual trap is the probability that a molecule that has flown into the trap will hit a cryogenic element and be condensed on it.

The coefficient of self-contamination ρ is the probability that a molecule that has escaped from the surface of an object placed in the chamber will return to that object.

The shielding coefficient β is the probability that a photon emitted by the object will hit the cryogenic elements of the pump system and be absorbed there.

The shielding coefficient serves to determine the degree of protection of the cryogenic elements from thermal radiation. Although this parameter does characterize the vacuum properties of the pump, the designer is almost always interested in the values of both parameters at once. Calculation of the coefficient β is similar to that of the parameter α, so we shall not describe it below.

Statistical Simulation and Characteristics of its Computer Realization. To calculate the above parameters by statistical simulation, we must know the geometry of the chamber and the local laws of behavior of a gas molecule. The following local laws were used in the calculation:

1) diffusive law of radiation of the source surface: the number of molecules emitted in direction l is proportional to the cosine of the angle φ between l and the normal n to the surface at the emission point;

2) diffusive law of reflection (independent of the angle of incidence of the molecule);

3) the free path is limited only by the chamber walls (sufficiently high vacuum); and

4) molecules are condensed with a probability of 1 on the cold (for a given gas component) shields and not at all on the warm shields.*

The velocity of a molecule in each rectilinear segment of its trajectory can also be simulated, but it is difficult to consider the local laws (accommodation coefficient, etc.) to be known here. It is advisable, therefore, to trace the motion of a molecule with constant velocity, the value of which is taken as 1 for convenience. Thus, the mean path $\bar{l}$ is determined. If the mean lifetime of a molecule must be obtained, then $\bar{t} = (1/\bar{v})\, \bar{l}$.**

Now let us describe the statistical simulation, which in our problem comes down to tracing the possible "life" path of molecules from the moment of escape to absorption. If we assume the absence of interaction between molecules, we can trace the trajectory of each molecule independently of the rest.

The trajectory of a molecule begins on the surface of the source. The points of escape are chosen randomly, according to the radiation density of the source surface. The direction of escape is chosen randomly from the set of possible directions, which are weighted in accordance with the diffusive law of radiation.

We determine the first rectilinear segment of the trajectory, i.e., we find the point of impact of the molecule against one of the chamber surfaces. The molecule can be either condensed or reflected at the impact point, depending upon the physical properties of the surface. By analyzing the physical properties of

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*Since molecular conditions are being considered, the concentration can differ from point to point.

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*In calculating β it should be assumed that when a photon hits the shield it is absorbed with probability ε, where ε is the blackness coefficient of the shield.

**We made a complete simulation with allowance for the local laws of variation of molecular velocity; this is also sequenced in real time on the M-20 computer.

the surface, we can determine the future behavior of the molecule.

If the molecule is condensed, this fact is recorded, the information required for further calculations is put down, and tracking of another molecule is begun.

If the molecule is reflected, the next segment of the trajectory is determined from the reflection law and the trace is continued.

Some molecules may wander too long in the chamber without being absorbed. To make the tracing of any particle final, we place an upper limit on the number of reflections. If a molecule undergoes ν reflections and is not absorbed, we stop tracing it and move to the next molecule. This, of course, increases the error of the method.

Having traced the trajectories of N molecules, we obtain the following information:

the lifetime t_i of the i-th molecule;

the path l_i of the i-th molecule;

the residence time Δt_i of the i-th molecule in isolated volume ΔV;

the path Δl_i traveled by the i-th molecule in volume ΔV;

the number n_ρ of molecules that have returned to the object; and

the number ΔN of molecules that have undergone ν reflections.

The values t_i and Δt_i are recorded when the local variation of molecule velocity is also simulated.

The number n_α of molecules absorbed by a trap is recorded for calculation of the capture coefficient of the trap.
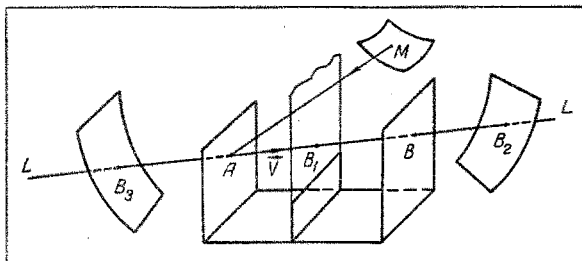

Fig. 2. Finding the next segment of the molecular trajectory.

The parameters that were defined above as means of random values are approximately equal to the arithmetic mean of the observed values in N tests:

$$\bar{t} = \frac{1}{N} \sum_{i=1}^{N} t_i; \quad \bar{l} = \frac{1}{N} \sum_{i=1}^{N} l_i;$$

$$\overline{\Delta t} = \frac{1}{N} \sum_{i=1}^{N} \Delta t_i; \quad \overline{\Delta l} = \frac{1}{N} \sum_{i=1}^{N} \Delta l_i. \qquad (9)$$

The parameters that were defined as probabilities of events are approximately equal to the frequencies of these events in N tests:

$$\alpha = \frac{n_\alpha}{N}; \quad \rho = \frac{n_\rho}{N}. \qquad (10)$$

The ratio $\Delta N/N$ should be taken into account in estimating the accuracy of the calculation results. We
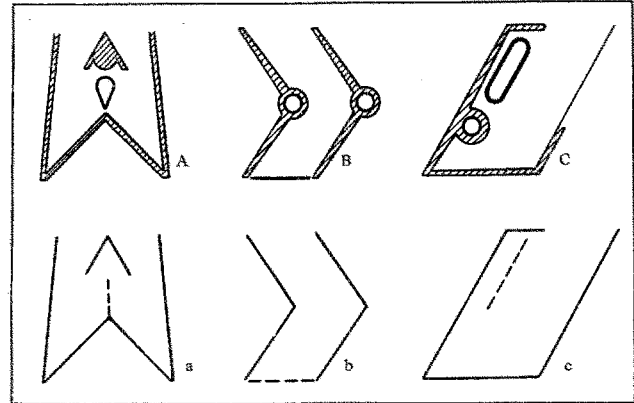

Fig. 3. Actual trap designs (A, B, and C) and their schematic representations (a, b, and c).

did not estimate the accuracy by the usual statistical tests; the calculation was stopped if stability was observed in the appearance of a given number of significant figures.

The proposed method for calculating the parameters can be carried out without using a high-speed computer. The calculations were made on a computer with a speed on the order of 20 000 operations per second.

The random laws were simulated by the conventional method (using a pseudorandom-number generator), which is described, for example, in [7].

The input data on the chamber geometry were written as follows: the surfaces were given by equations in a fixed Cartesian coordinate system and the necessary regions on these surfaces were isolated by a special system of inequalities. Each surface was given a sign, which coded its physical properties.

The simulation program was written so that it did not require changes when a new chamber with different geometry was calculated; only data on the geometry and physical properties of the surfaces of the new chamber need be entered. This program universality was achieved as a result of a uniform method of tracing molecule trajectories. The method is explained in greater detail with the aid of Fig. 2.

Table 1

Values of l for Sphere with Diffuse Radiation

N	2000	6000	10000	14000	18000	30000	Theoretical value
$\bar{l}$	8.53	8.19	8.34	8.35	8.40	8.44	8.49

Table 2

Values of l for Sphere with Uniform Radiation

N	2000	4000	6000	10000	18000	25000	Theoretical value
$\bar{l}$	7.07	6.77	6.73	6.73	6.69	6.66	6.67

Let a molecule arrive at point A from point M (previous step) and let it be required to determine the next segment of its trajectory, i.e., the segment AB.

Table 3

Capture Coefficients α for Actual and Schematic Traps

Diagram	Number of tests							
	1000	3000	5000	6000	7000	8000	9000	10000
Fig. 3,A	0.247	0.248	0.242	0.243	0.246	0.248	0.248	0.246
Fig. 3,a	0.272	0.284	0.278	0.278	0.281	0.284	0.282	0.281
Fig. 3,B	0.250	0.244	0.238	0.238	0.241	0.241	0.241	0.241
Fig. 3,b	0.300	0.302	0.291	0.292	0.293	0.293	0.292	0.290
Fig. 3,C	0.524	0.516	0.519	0.518	0.516	0.515	0.518	0.517
Fig. 3,c	0.468	0.472	0.477	0.475	0.473	0.475	0.475	0.473

We represent the equation of line L in parametric form:

$$x = x_0 + v_x t, \quad y = y_0 + v_y t, \quad z = z_0 + v_z t, \tag{11}$$

where x_0, y_0, and z_0 are the coordinates of point A and $v = (v_x, v_y, v_z)$, which is obtained by simulation of the corresponding laws. The sense of the velocity vector is given by the condition

$$(\mathbf{AM}, \ \mathbf{n}) \cdot (\mathbf{v}, \ \mathbf{n}) > 0, \tag{12}$$

where n is the normal to the surface at point A. Condition (12) means that **AM** and **v** are on the same side relative to the normal.* The points of intersection of line L with the surfaces are found by solving Eq. (11) jointly with the equations of the surfaces. The required point (point B) is found by sorting all points and eliminating the extraneous ones by means of a system of checks. In the first place, points that do not belong to the isolated regions are eliminated (point B_1 in Fig. 2 would be eliminated by this criterion). Then, the points that lie in the opposite direction of the flight of the molecule are eliminated. These points would correspond to negative collision times, since the velocity vector obeys condition (12). In Fig. 2, this is point B_3. From the remaining points we select the one closest to point A, which will be the desired point (point B).

There are special cases in which more economical simulation is possible. In determining the capture coefficient, it is often sufficient to consider a two-dimensional rather than a three-dimensional model of a trap or chamber. This simplifies the writing of input data and reduces computation time. In this case, the calculation is performed by a separate program.

In calculating designs with periodic elements, it is sufficient to indicate only one standard segment and the means of its periodic continuation. This simplifies calculation of the parameters of open traps, i.e., those with outputs not only to the working space of the chamber but also to adjacent traps. The amount of input data can also be reduced when the parameters of traps with a symmetry plane are calculated. In this case, it is sufficient to describe only half of the trap and to code the symmetry plane as a surface with mirror reflection.

Statistical-simulation programs have about one thousand triple-address instructions. The computation time is a function of the complexity of the geometry and of the desired accuracy. In the following section, we shall give examples of calculation of several design versions, which will allow the effectiveness of the method to be judged.

Mean Path of Molecule in Spherical Chamber. To get an idea of the accuracy obtained when the parameters are calculated by the Monte Carlo method, let us compare the results of computer calculation with the exact values for a spherical chamber. Formulas (15) and (16), below, are also of interest for rough calculations of the parameters of complex chambers.

We shall consider a spherical chamber of radius R on the inside surface of which is placed a point source with a diffusive law of radiation.* The chamber surface reflects molecules with probability γ, and reflection is also diffuse. We shall be interested in the mean path of a molecule $\bar{l}$. For the random value l (path) we can write the equation

$$l = d + Al, \tag{13}$$

where d is the length of the first segment of the trajectory and A is a random value that takes on values of 1 and 0; a probability of 1 equals γ. Converting to mean values in (13), we obtain $\bar{l} = \bar{d} + \gamma \bar{l}$; hence,

$$\bar{l} = \frac{\bar{d}}{1 - \gamma}. \tag{14}$$

It remains to calculate $\bar{d}$, i.e., the mean length of the chords drawn from the radiation point according to the diffusion law. Standard calculation gives $\bar{d} = 4R/\pi$,

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*With the escape of a molecule, the direction is selected by means of the normal to the surface of the source, which must be oriented to the required side.

*The following diffusive law is assumed: angles Θ and φ, which determine the direction of flight of the molecule, are distributed uniformly on the intervals $[10, \eta/2]$ and $[0, 2\pi]$, respectively.

Table 4

Parameter Values for Cylindrical Chambers

Diagram and parameters		Number of tests						
		100	500	1000	1500	2000	2500	2700
Fig. 4a	$\bar{l}$	92.91	94.53	95.30	96.13	96.00	95.50	95.20
	$\overline{\Delta l}$	0.036	0.052	0.042	0.040	0.047	0.051	0.050
	ρ	0.56	0.51	0.49	0.50	0.50	0.51	0.51
Fig. 4b	$\bar{l}$	71.16	68.01	67.90	67.73	67.51	67.40	67.41
	$\overline{\Delta l}$	0.026	0.041	0.034	0.036	0.034	0.034	0.033
	ρ	0.44	0.39	0.38	0.39	0.38	0.39	0.39

which, substituted into (14), gives

$$\bar{l} = \frac{4R}{\pi(1-\gamma)}. \qquad (15)$$

Computer results for $R = 2$ and $\gamma = 0.7$ are shown in Table 1. Similar results for a source with uniform radiation (equal numbers of molecules in all directions) are given in Table 2. In the case of a uniformly emitting source, for the mean path $\bar{l}$ we have

$$\bar{l} = \frac{R}{1-\gamma}. \qquad (16)$$

Capture Coefficient of the Trap. Figure 3 shows cross sections of traps for which the capture coefficient α was calculated. The proposed method makes it possible to estimate the extent to which the values of the parameter α differ when calculated for the actual and schematic traps. In Fig. 3, the relative dimensions of the trap elements for which the coefficients α were computed are maintained. The cryogenic elements are shown by solid lines in the actual designs and by dashed lines in the schematics.

The calculation results are given in Table 3. The calculation was made for a two-dimensional trap model. It was assumed that the points of entry of molecules into the trap were uniformly distributed on the input line and at each point the direction of entry is taken from the projection of the diffusive law of radiation onto the plane.

Parameters for Cylindrical Chambers. Let us consider two chambers that are open circular cylinders. Cylindrical objects are placed on the axes of the cylinders; the height of the object equals the chamber height. Cross sections of the chambers are shown in Fig. 4, in which the cryogenic elements of the traps are indicated by dashed lines. Molecules are absorbed by the cryogenic elements with a probability of 1. In the simulation it was assumed that the trajectory of a molecule ended when it hit a cryogenic element or the surface of the object.

Table 4 shows the calculation results for the mean path $\bar{l}$ of molecules in the chamber, the mean path $\overline{\Delta l}$ of molecules in isolated volume ΔV, and the self-contamination coefficient ρ. It was assumed that the points of escape of the molecules were uniformly distributed over the surface of the object and that the directions of escape were distributed in space according to the diffusive law. The reflection of molecules was diffusive. In Fig. 4, the relative dimensions

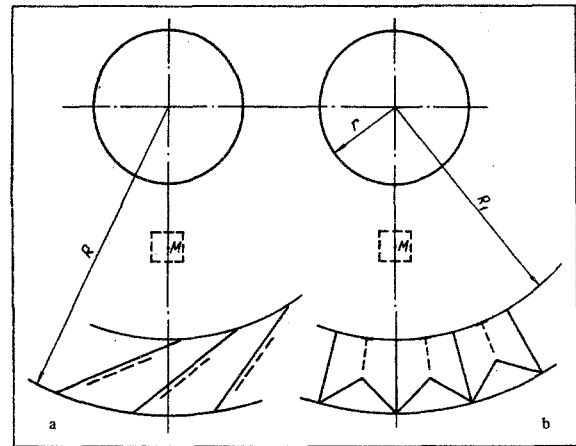of the chamber elements correspond to the dimensions of the calculated designs.

Fig. 4. Cross sections of cylindrical chambers: $R = 20$ cm; $R_i = 15$ cm; $r = 5$ cm; chamber height $h = 60$ cm.

NOTATION

$\bar{N}_c$ is the number of molecules in the chamber under steady-state conditions; q and r are the source and discharge intensities, respectively; $\bar{n}_0$ is the mean concentration of the molecules in the chamber; $n(M)$ is the local concentration of the molecules at point M of the chamber; S is the pumping rate; $\bar{t}$ is the mean lifetime of the molecules in the chamber; $\bar{l}$ is the mean path of the molecules in the chamber before absorption; $\overline{\Delta t}$ and $\overline{\Delta l}$ are, respectively, the mean residence time and the mean path of the molecule in an isolated volume ΔV; α is the capture coefficient of the trap; β is the shielding coefficient of the cryogenic elements; ρ is the self-contamination coefficient of the object; N is the number of tests.

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