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Calculation of time-dependent pressure under molecular flow using Monte Carlo method

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ABSTRACT

The Monte Carlo method can be used to study the time-dependent pressure in a vacuum system. In the usual simulation process, the test particles are traced and the locations of them are recorded at certain times, while they move and bounce in a vacuum chamber. So the particle numbers at some locations and moments can be obtained and then transformed into pressures using the ideal gas equation. A new method based on Monte Carlo is proposed in this paper. The locations and moments of the collisions between the particles and inner walls of chamber are calculated firstly, and then the locations of the particles at any other time are obtained by interpolation. For simplicity, pressure evolution in a pipe with rectangular cross section is simulated and presented to state this method.

1. Introduction

Calculation of pressure distribution in a vacuum system is a classical problem in vacuum science and of great practical importance [1]. It is usually difficult to get the analytical solution, especially for the systems with complex shapes. The Monte Carlo method, first applied to vacuum science by Davis [2], has been widely used in various fields such as conductance or transmission probability calculation of vacuum pipes [3,4], design of vacuum pumps [5,6], and pressure distribution in vacuum systems [1]. Suetsugu applied this method to calculation of the time-dependent pressure distribution [7]. In that paper, the test particles are traced and locations of them are recorded at certain times, so the particle densities and thus the pressures in the vacuum system at those times can be obtained. A different method is proposed in this paper and described in detail below.

2. Simulation method

To state the simulation method and processes, a strait pipe with rectangular cross section, as shown in Fig. 1, is employed for simplicity. The pipe is composed of two parts with different cross sectional dimensions (denoted by I and II). The width, height and length of the two parts are 50, 50, 150 mm and 100, 100, 150 mm respectively. For ease of pressure calculation and display, the two parts are divided into two grids of 20 × 20 × 30 and 40 × 40 × 30 cubic cells of equal size (2.5 × 2.5 × 5 mm) respectively.

The involved parameters and their values in the simulation are listed in Table 1. In a real vacuum system, the gas source can be mainly divided into two parts: the injected gas from the inlet and the desorbed gas from the walls of vacuum system. Because the molecules don't affect each other, the pressure induced by the injected and desorbed gas can be calculated separately and the total pressure is the sum of them. The rates of gas injection and desorption Q are 1.0×10^{16} s^{-1} and 1.0×10^{14} s^{-1} (number of molecules injected and desorbed per second), i.e., 3.78×10^{-2} Pa L/s and 3.88×10^{-7} Pa L/(s cm^2), respectively. The velocities of the molecules v follow Maxwell distribution:

$$f(v) = 4\pi v^2 \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} e^{-\frac{mv^2}{2kT}} \quad (1)$$

The number of molecules even in high vacuum is so large that the Monte Carlo simulation is impractical for the present personal computer. Therefore, to reduce the amount of calculation, one test particle in the simulation usually represent a crowd of real molecules, which is $n_m = 2.5 \times 10^5$ for the injected gas and 2.5×10^3 for the desorbed gas. In the duration of gas injection and desorption, the particles are assumed to enter the chamber one by one, so the

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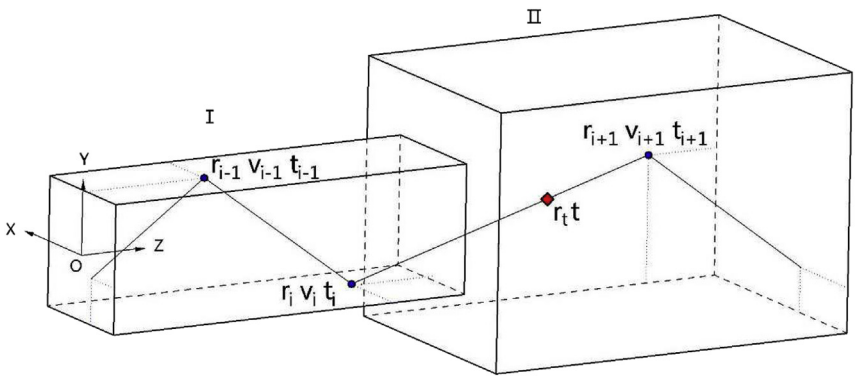

Fig. 1. The geometric model of the simulation.

Table 1
Parameters involved in the simulation.

Parameter		Value
k	Boltzmann constant	1.38×10^{-23} [J/K]
NA	Avogadro's constant	6.02×10^{23} [mol^{-1}]
T	Temperature	293 [K]
m	Molecular mass	29/NA [g]
v	Molecular velocity	Maxwell distribution
Q	Gas injection and desorption rate	1.0×10^{16} [s^{-1}] 1.0×10^{14} [s^{-1}]
t_d	Gas injection duration	0.025 [s]
n_m	Molecules corresponding to one test particle	2.5×10^5 2.5×10^3
N_s	Number of test particles	$Q\ t_d/n_m$
Δt	Time interval of entrance	n_m/Q [s]
t_r	Residence time on the surface	0, 0.1, 0.5 ms

entry time interval of two consecutive particles is $\Delta t = n_m/Q$, i.e., 2.5×10^{-11} and 2.5×10^{-13} s. A large number of particles, $N_s = 1.0 \times 10^9$ here, are generated to insure the statistic accuracy.

Similar to the usual Monte Carlo calculation, the simulation in this paper is performed under the following assumptions:

(1) The molecules injected from the inlet and desorbed from the inner walls of the system, while entering into the vacuum system in question, are distributed uniformly on the entrance and the inner surface respectively, with a distribution of directions according to cosine law.
(2) The gas flow is assumed to be molecular, i.e. the intermolecular collisions are neglected.
(3) The reflection of molecules from the walls of the system is diffuse and the accommodation coefficient is one, i.e. the directions and velocities after the reflections follow the cosine law and Maxwell distribution respectively.
(4) The molecules can move to the gas inlet after multiple reflections with the walls, and then be reflected from the inlet immediately. The locations and directions of them are defined according to assumption (1). The molecules will exit the vacuum system once arriving at the outlet, i.e. sticking coefficient of the outlet is one.

The procedure of the simulation is shown Fig. 2. After parameter initializing, the test particles enter into the pipe from the inlet and the inner walls, and the entry time of the nth particle is $(n-1)\ \Delta t$. Then the coordinates $r_i (i = 1, 2, \ldots)$ or (x_i, y_i, z_i), where the particles collide with the walls of the pipe, are calculated by solving these equations:

$$\begin{cases} x_i = \pm\dfrac{W}{2},\ \ y_i = \pm\dfrac{H}{2} \\ \dfrac{x_i - x_{i-1}}{\alpha_{i-1}} = \dfrac{y_i - y_{i-1}}{\beta_{i-1}} = \dfrac{z_i - z_{i-1}}{\gamma_{i-1}} \end{cases} \tag{2}$$

where $(x_{i-1}, y_{i-1}, z_{i-1})$ is the last collision point, and $(\alpha_{i-1}, \beta_{i-1}, \gamma_{i-1})$ is the last direction cosine. There are four set of solutions, but only one is appropriate and adopted, considering the motion direction of the test particles. The velocities of the test particles are generated in accordance with the Maxwell distribution by:

$$v_i = \sqrt{\frac{-3kT \ln \varepsilon}{m}} \quad if\ \ \eta^2 < -e\varepsilon \ln \varepsilon \tag{3}$$

where ε and η are random numbers chosen uniformly between 0 and 1. The corresponding motion distance and time moment are:

$$s_i = |r_{i+1} - r_i| \tag{4}$$

$$t_{i+1} = t_i + \frac{s_i}{v_i} \tag{5}$$

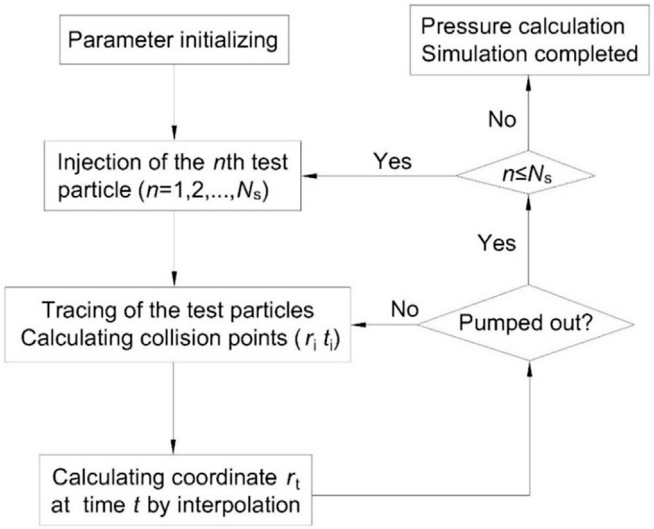

Fig. 2. The program flow chart of the simulation.