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Using Plücker Coordinates for Pumping Speed Evaluation of Molecular Pump in the DSMC Method

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In this study, the Plücker coordinates representation is used to formulate the ruled surface and the molecular path for pumping speed performance evaluation of a molecular vacuum pump. The ruled surface represented by the Plücker coordinates is used to develop a criterion for when gas molecules hit the pump surface wall. The criterion is applied to analyze the flow rate of a new developed vacuum pump in transition regimes by using the DSMC (Direct Simulation Monte Carlo) method. When a molecule flies in a neutral electrical field its path is a straight line. If the molecular path and the generators of a ruled surface are both represented by the Plücker coordinates, the position of the molecular hit on the wall can be verified by the reciprocal condition of the lines. The Plücker coordinates representation is quite convenient in the DSMC method for this three-dimensional molecular flow simulation.

Keywords: Vacuum pump, DSMC method, Plücker coordinates

1 INTRODUCTION

In a high vacuum, gas molecules are rarefied and cannot be regarded as a continuum. The state of gas flow is analyzed based on the kinetic theory for rarefied gas. The kinetic model is governed by the Boltzmann equation

$$\frac{\partial}{\partial t}(nf) + \vec{c}\cdot\frac{\partial}{\partial \vec{r}}(nf) + \vec{F}\cdot\frac{\partial}{\partial \vec{c}}(nf) = \int_{-\infty}^{\infty}\int_{0}^{4\pi} n^2(f^*f_1^* - ff_1)c_r\sigma\,\mathrm{d}\Omega\,\mathrm{d}\vec{c}_1. \quad (1)$$

The right hand side of this equation expresses the collision term of molecules, in which a molecule of

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class c has a collision with one of class c_1. Where, the vector $\vec{r}$ is the molecular position, $\vec{c}$ denotes the molecular speed, and $\vec{F}$ indicates the force vector. Based on the probability distribution, n is the number density of molecules, f is single particle distribution function in velocity space, and nf is single particle distribution function in phase space. As f denotes the velocity distribution function at class c, f_1 is the value of f at c_1. In the collision term, Ω is the solid angle of molecular collision, σ is the collision cross-section, c_r is the relative velocity of molecules, and the superscript $*$ denotes the post collision.

To solve the Boltzmann equation is quite complex, and huge numerical computations are required to solve rarefied gas kinetics based on the Boltzmann equation. The most commonly used numerical method in rarefied gas kinetics is the Direct Simulation Monte Carlo (DSMC) method. Bird (1976) developed the DSMC method for rarefied gas analysis. At that time, it was widely applied in aerospace engineering. Recently, it gains a lot of attention on the application of microelectronics, microelectromechanical system (MEMS), and vacuum technology (Nanbu, 1996). For the development of the vacuum pump, it was successfully applied on the diffusion pump (Lee and Lee, 1996), cryopump (Akiyama *et al.*, 1971), and molecular pump (Nanbu *et al.*, 1991). The DSMC method is an effective tool in the design of vacuum devices, such as the vacuum pump, sputtering apparatuses, plasma chamber, and so on. It plays an important role in the development of semiconductor manufacturing devices.

The flow regime is determined by the Knudsen number, Kn, that is defined by

$$Kn = \frac{\lambda}{D}, \tag{2}$$

where λ is the molecular mean free path, and D is the characteristic length. The kinetic theory is applied if the Knudsen number satisfies

$$Kn > 0.01. \tag{3}$$

When $Kn > 0.01$, the gas flow is recognized as rarefied gas, and the DSMC method is employed. For $Kn \ll 0.01$, the gas flow is regard as a continuum, and the Navier–Stokes equation is applicable.

As shown in Fig. 1, the approach of the DSMC method is to the trajectories of a very large number of simulated molecules simultaneously for a small time interval. The molecular motion and the intermolecular collisions are treated separately. All of the molecules are moved over the distances appropriate to the time step, which is chosen to be much smaller than the mean collision time. The resulting boundary interactions are calculated during the time interval. Then it is followed by the calculation of intermolecular collisions in this time step. The representative sets of collisions are selected through

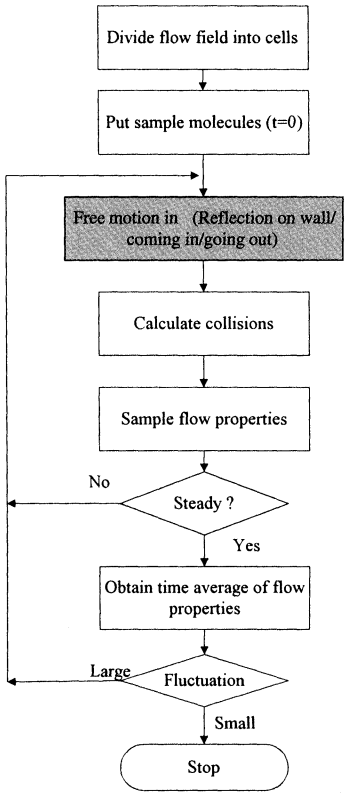

FIGURE 1 Flow chart of DSMC.

the probabilistic procedures which are based directly on the kinetic theory and therefore under the assumption of molecular chaos as well as the requirements of a dilute gas. The proper physical space cell network is required when choosing the collision sets, and sampling the macroscopic flow properties. In the present work, we examine the flow of a new developed pump in the molecular and transition regimes by the DSMC method.

For the free motion of a sample molecule, the molecular path is a simple straight line. In a free molecular flow regime, $Kn \gg 0.01$, the molecular mean free path is much larger than the characteristic length of the vessel. The collisions between molecules are neglected. All the collisions are assumed to be between the molecules and the surface wall. Considering the molecular reflection on the wall, it can be seen that reflections, such as diffuse or specular reflections, are dependent on the reflection model. As shown in the third process of Fig. 1, the position of molecules hitting the wall should be found before calculating reflection in the DSMC method. Finding the hitting positions is an analytical geometric problem. As shown in Fig. 2, if a molecule passes through a point (x_1, y_1, z_1) with the velocity (v_x, v_y, v_z), the path line is represented as a parametric form

$$\vartheta(t) = \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} + t \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} \tag{4}$$

and the surface of the apparatus wall is written as an implicit form

$$F_s(x, y, z) = 0. \tag{5}$$

The hitting positions are obtained by substituting Eq. (4) to (5). Unfortunately, the implicit form of Eq. (5) is not so easily obtained. The approximate wall boundary is usually constructed by shrinking the cells near the wall (Nanbu and Fukumoto, 1993). The hitting positions are obtained by substituting the approximate surface. In this paper, a convenient rule is developed to find hitting position based on the Plücker coordinates and the line geometry.

2 RULED SURFACE

A ruled surface, as shown in Fig. 3, is a surface constructed by a family of line segments in three-dimensional space. It is the locus of the line segments in space with four degrees of freedom. It is a common geometric entity in machine parts. Cylinders, cones, helicoids, and hyperloids are all typical ruled surfaces. The majority of three-dimensional machine parts are mostly composed of ruled surfaces. In general, a ruled surface is expressed as the parametric form

$$\mathbf{r}(u, t) = \mathbf{r}(u) + t\,\underline{\mathbf{v}}(u), \tag{6}$$

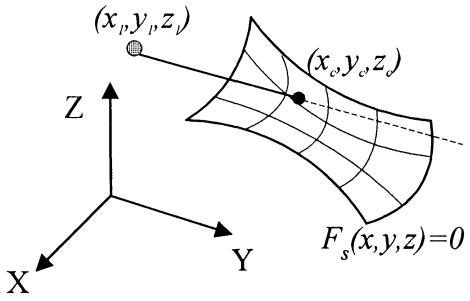

FIGURE 2 Free molecular motion and hitting position on wall.

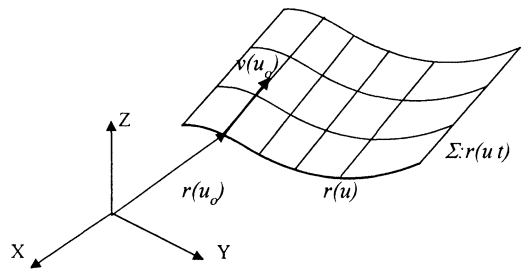

FIGURE 3 A ruled surface defined by a directrix and ruling vector.

where $\mathbf{r}(u)$ is a spatial curve named directrix, $\underline{\mathbf{v}}(u)$ is a ruling vector, $u_i < u < u_f$, $t_i < t < t_f$. The lines in a ruled surface are called generators and the parameter t represents the length of the line segment. Also, the ruled surface can be defined by two directrixes. It is represented as

$$\mathbf{r}(u, t) = \mathbf{r}_1(u) + t[\mathbf{r}_1(u) - \mathbf{r}_2(u)], \tag{7}$$

where $\mathbf{r}_1(u)$ and $\mathbf{r}_2(u)$ are directrixes.

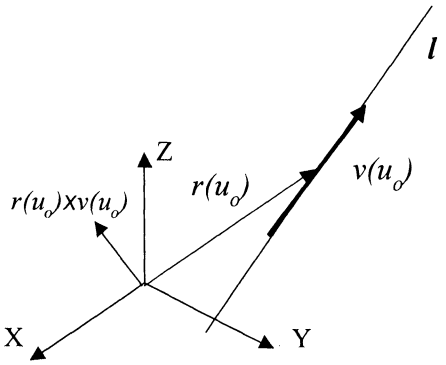

FIGURE 4 A line in three-dimensional space.

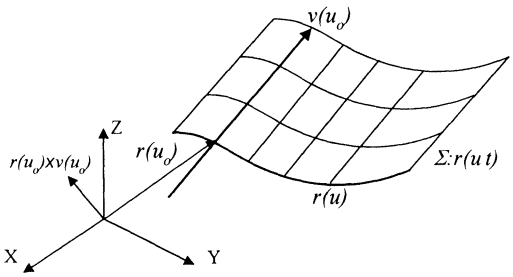

FIGURE 5 Ruled surface defined by a straight line and plücker coordinates.

2.1 Plücker Coordinates

A line in three-dimensional space is usually represented as the parametric form

$$l: \quad \mathbf{r}(t) = \mathbf{r}(u_0) + t[\underline{v}(u_0)], \quad t \in \{-\infty, \infty\}, \tag{8}$$

where $\mathbf{r}(u_0)$ is an arbitrary position on the line, and $v(u_0)$ is the direction cosine of that line. The Plücker coordinates, with six elements, are purely geometric. They represent a point in a six-dimensional projective five space; and its projection in three-dimensional space is a straight line with an associate scalar pitch. The six elements of the Plücker coordinates are $[L, M, N, P, Q, R]$. For the normalized Plücker coordinates, the constraint $L^2 + M^2 + N^2 = 1$ should be satisfied. In Euclid geometric space, $[L, M, N]$ is the direction cosine of the line, and $[P, Q, R]$ is the moment of that line about the reference frame origin. As shown in Fig. 4,

$$\underline{v}(u_0) = \begin{bmatrix} L \\ M \\ N \end{bmatrix} \quad \text{and} \quad r(u_0) \times \underline{v}(u_0) = \begin{bmatrix} P \\ Q \\ R \end{bmatrix}.$$

Hence, a straight line in three-dimensional space is represented by

$$l: \quad l = \begin{bmatrix} \underline{v}(u_0) \\ r(u_0) \times \underline{v}(u_0) \end{bmatrix} = [L \; M \; N \; P \; Q \; R]^{\mathrm{T}}. \tag{9}$$

Not only can the Plücker coordinates represent straight lines but also screws in Euclid space. Generally speaking, a line is a screw of zero pitch. It should meet the quadratic identity, QI.

$$QI: \quad LP + MQ + NR = 0. \tag{10}$$

The quadratic identity constrains the six-dimensional Plücker coordinates to be a zero pitch line.

2.2 Ruled Surface with Plücker Coordinates

In a ruled surface, the generators can be expressed by the Plücker coordinates. As shown in Fig. 5, $r(u)$ is the directrix and $v(u)$ are the ruling vectors. A generator l_{u0} is represented as the parametric form of Eq. (8), and the ruled surface Σ is represented

as Eq. (6). In the Plücker coordinates, l_{u0} is expressed as

$$l: \quad l_{u0} = \begin{bmatrix} \underline{v}(u_0) \\ r(u_0) \times \underline{v}(u_0) \end{bmatrix} = [L_{u0}\ M_{u0}\ N_{u0}\ P_{u0}\ Q_{u0}\ R_{u0}]^{\mathrm{T}}$$

and the ruled surface Σ is formulated as

$$\Sigma: \quad S(u) = \begin{bmatrix} \underline{v}(u) \\ r(u) \times \underline{v}(u) \end{bmatrix} = [L(u)\ M(u)\ N(u)\ P(u)\ Q(u)\ R(u)]^{\mathrm{T}}, \tag{11}$$

where $r(u)$ is the directrix. The boundary of the ruled surface can be found by

$$r_A(u) = r(u) + t_A \underline{v}(u), \quad r_B(u) = r(u) + t_B \underline{v}(u), \tag{12}$$

t_A and t_B are functions of u.

3 MOLECULAR PATH AND HIT POSITION ON A RULED SURFACE

A molecule in free molecular flow flies along a straight line until the molecule hits a surface wall. The Plücker coordinates can formulate the molecular path. Assuming a molecule, which has a velocity of $\vec{v} = (v_x, v_y, v_z)$, locates on $\vec{r} = (x, y, z)$. In the next step, after the time interval t, the molecule will move to (x', y', z'). The path line of this molecule in parametric form is then

$$\vartheta(t) = \begin{bmatrix} x + v_x t \\ y + v_y t \\ z + v_z t \end{bmatrix}.$$

It can also be represented as the normalized Plücker coordinates

$$\vartheta: \quad \frac{1}{\|\vec{v}\|} \begin{bmatrix} \vec{v} \\ \vec{r} \times \vec{v} \end{bmatrix} = \frac{1}{\|\vec{v}\|} [v_x\ v_y\ v_z\ yv_z - zv_y\ zv_x - xv_z\ xv_y - yv_x]^{\mathrm{T}}. \tag{13}$$

The reciprocal product of two lines in Plücker coordinates, $\vartheta_1 = (L_1, M_1, N_1, P_1, Q_1, R_1)^{\mathrm{T}}$ and $\vartheta_2 = (L_2, M_2, N_2, P_2, Q_2, R_2)^{\mathrm{T}}$, is

$$\vartheta_1 \circ \vartheta_2 = L_1P_2 + M_1Q_2 + N_1R_2 + P_1L_2 + Q_1M_2 + R_1N_2. \tag{14}$$

It is the geometric relationship of these lines. In geometry, it is equal to

$$\vartheta_1 \circ \vartheta_2 = -d \sin\alpha, \tag{15}$$

where d is the distance along the common perpendicular line and α is the angle of ϑ_1 and ϑ_2 respectively. If two lines are intersected, the reciprocal product is equal to zero. Hence, the reciprocal condition is the necessary condition for a molecule hitting a generator on a ruled surface wall. Considering the special case of two parallel lines, the angle α is equal to zero, and their intersection is recognized as infinite. From the geometric relationship, the intersection of molecules and generators on a ruled surface wall are easily found.

Molecular hitting occurs at a specified generator on the ruled surface. The parameter, u_0, of this generator should meet the reciprocal condition

$$S(u_0) \circ \vartheta = 0. \tag{16}$$

The generator, $l(u_0)$, which has an intersection with the path line is

$$l(u_0) = \begin{bmatrix} \underline{v}(u_0) \\ r(u_0) \times \underline{v}(u_0) \end{bmatrix} = [L(u_0)\ M(u_0)\ N(u_0)\ P(u_0)\ Q(u_0)\ R(u_0)]^{\mathrm{T}}.$$

Then the hitting position $x(t_0)$ is the intersection of $l(u_0)$ and ϑ. And $x(t_0)$ should be within the boundary of the ruled surface, i.e. $t_A \le t_0 \le t_B$ in Eq. (12). In spite of the necessary reciprocal condition, the boundary limitation is the sufficient condition for molecule collision on the wall.

Consider the reflection model, excepting the random diffuse reflection, the surface normal should be obtained after finding the hitting position. In a ruled surface, points on a generator have a unique surface normal. The surface normal is

obtained by the cross product of the directrix tangent and the generator direction.

$$n(u) = \frac{\mathrm{d}r(u)}{\mathrm{d}u} \times \underline{v}(u). \tag{17}$$

4 ANALYSIS OF A NEWLY DEVELOPED VACUUM PUMP

4.1 Surface Construction

The geometry of the newly developed molecular pump is a high rotational speed rotor with five variable pitch screw threads and variable groove depth. Along the axial direction, the rotor is divided into ten regions from the inlet to the outlet. As shown in Fig. 6, rotor geometry is designed by the turbo molecular pump (TMP) criteria in the *first* region. From the *third* to *tenth* regions, the dimension is determined based on a molecular drag pump with spiral grooves (Sawada and Nakamura, 1985). And the second region is a transition region, which connects the first stage to the third stage. The helix angle is a constant in each region. In Fig. 7, a solid model is generated by the geometric parameters. The top view and the front view of the rotor are also shown in this figure.

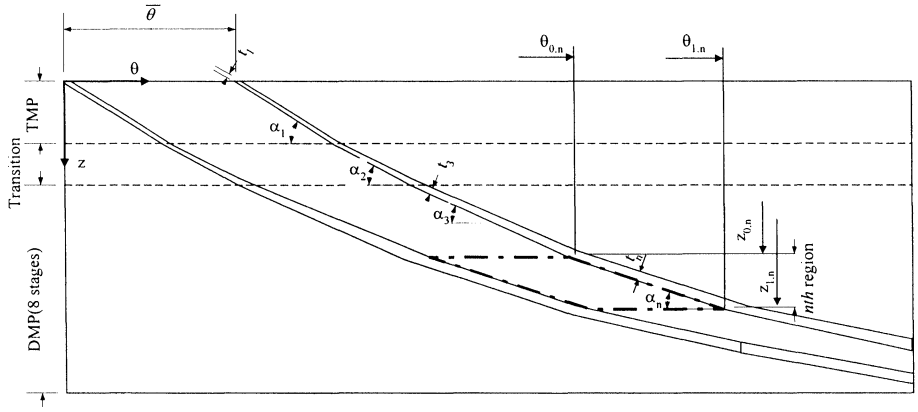

FIGURE 6 Auxiliary projective drawing of rotor geometry.

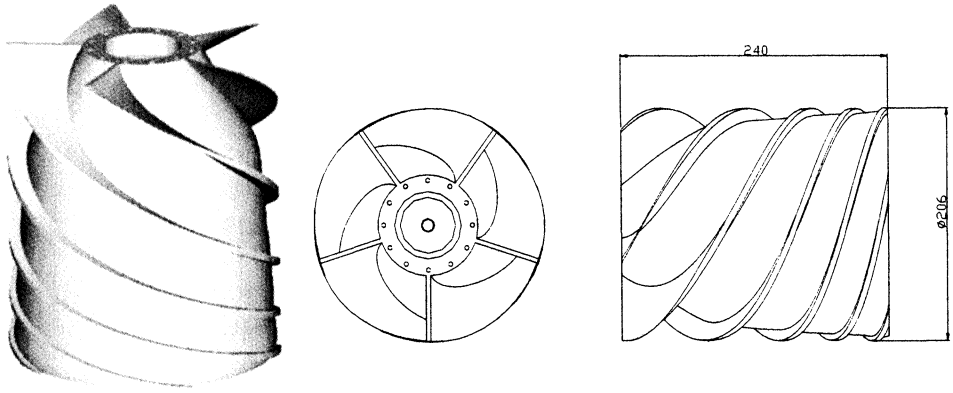

FIGURE 7 A variable pith screw thread rotor.

The variable pitch screw threads and ditches are all ruled surface. The directrix for a thread in the nth stage is denoted as

$$\mathbf{r}(\theta) = \begin{bmatrix} r_h \cos\theta \\ r_h \sin\theta \\ z_{0,n} - \tan\alpha_n r_h(\theta - \theta_{0,n} - \bar{\theta}) \end{bmatrix} \tag{18}$$

and $\theta_{0,n} + \bar{\theta} \le \theta \le \theta_{1,n} + \bar{\theta}$, where $\bar{\theta}$ is the beginning revolution angle of a thread. The subscript n indicates the nth region, r_h is the outer diameter, α is the helix angle of thread, and θ is a parameter in the revolution angle. In nth region, a rotor thread is from $z_{0,n}$ to $z_{1,n}$ in the axial direction and a revolution from $\theta_{0,n}$ to $\theta_{1,n}$ about the axial direction. This directrix is a helical curve on the thread tip. Generator direction is $v(\theta) = [\cos\theta \sin\theta 0]^T$. In Plücker coordinates, the thread surface is represented as

$$S_t(\theta) = \begin{bmatrix} v(\theta) \\ r(\theta) \times v(\theta) \end{bmatrix} = \begin{bmatrix} \cos\theta \\ \sin\theta \\ 0 \\ r_h \sin\theta \tan\alpha_n(\theta - \theta_{0,n} - \bar{\theta}) - z_{0,n}\sin\theta \\ z_{0,n}\cos\theta - r_h \cos\theta \tan\alpha_n(\theta - \theta_{0,n} - \bar{\theta}) \\ 0 \end{bmatrix} \tag{19}$$

and its surface normal is

$$n(\theta) = \frac{dr(\theta)}{d\theta} \times v(\theta) = \begin{bmatrix} -\tan\alpha_n \sin\theta \\ \tan\alpha_n \cos\theta \\ 1 \end{bmatrix}. \tag{20}$$

Substituting Eqs. (13) and (18) into the reciprocal condition Eq. (16), the necessary condition for molecule hitting on the ruled surface wall, the hit position is then obtained by solving

$$\tan\theta = -\frac{A_0 + A_1\theta}{B_0 + B_1\theta}, \tag{21}$$

where

$$\begin{cases} A_0 = y_1 v_z - z_1 v_y + v_y r_h \tan\alpha_n(\theta_{0,n} + \bar{\theta}) + z_{0,n} v_y, \\ A_1 = -v_y r_h \tan\alpha_n, \\ B_0 = z_1 v_x - x_1 v_z + v_x r_h \tan\alpha_n(\theta_{0,n} + \bar{\theta}) + z_{0,n} v_y, \\ A_1 = -v_x r_h \tan\alpha_n. \end{cases}$$

When considering the molecular hit on the casing or ditch, it is not necessary to use the Plücker coordinates. Even the casing and cylinder are ruled surface, it is quite easy to find the collision position by an usual method which substitutes Eq. (4) to (5). The ditch is constructed by six cone surfaces. The cone surface in nth stage is $F_d(x, y, z) = x^2 + y^2 - r^2(z) = 0$ where $r(z) = r_{0,n} + (z - z_{0,n})/(z_{1,n} - z_{0,n}) \times (r_{1,n} - r_{0,n})$. The casing surrounding the rotor is a cylinder surface, which is represented as an implicit function $F_h(x, y, z) = x^2 + y^2 - r_h^2 = 0$.

4.2 Numerical Simulation by the DSMC Method

In the DSMC method the flow field in a groove is first divided into cells, as shown in Fig. 8. The cells are indicated by (i, j, k) along the radial direction r,

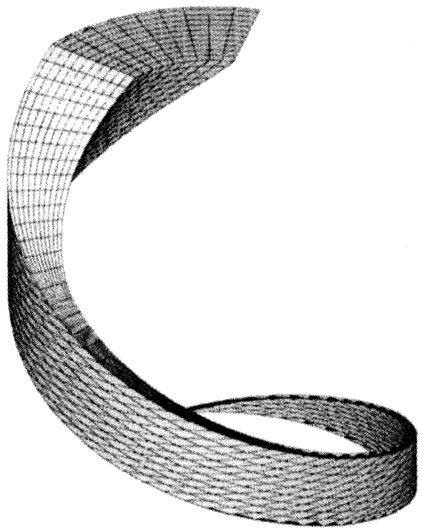

FIGURE 8 Cells construction in a variable pith screw grooved.

revolution θ, and axial direction z. The molecular inter collisions are calculated independently in each cell. The cells are also used to sample the macroscopic flow properties in the DSMC method.

The Plücker coordinates for formulating the rotor surface and molecular path are applied to the numerical simulation by the DSMC method. The flow field is a channel, which is one of the variable pitched rotor grooves. As shown in Fig. 1, the sample molecules are first introduced into the flow field. Then the molecular motion and collision are calculated until the fluctuation of flow properties is convergent. Using the Plücker coordinates in the DSMC method, the surface wall of pump thread is formulated by Eq. (19), and the molecular path is expressed as Eq. (13). As the third process of Fig. 1, the position of a molecule hitting the thread surface is located by solving Eq. (21), and the surface normal are obtained from Eq. (20) to deal with the molecular reflection.

The numerical simulation for pumping speed evaluation is shown as Fig. 9. Let the rotation speed be 24 000 rpm, the velocity at thread tip is about 260 m/s. When the inlet pressure and outlet pressures are given, the flow rate in a channel is obtained by the iteration of the DSMC method. Neglecting the characteristics of the foreline pump, let the outlet pressure be a constant 0.0133 mbar. The chosen pressure is a reasonable pressure for a dry vacuum pump or mechanical pump to be the foreline pump. To find the flow rate, let the inlet pressure be varied from 0.000133 to 0.0133 mbar. The throughput and pumping speed are plotted in Fig. 9(a) and (b) respectively.

In the inlet port, the flow regime is in transition flow. The Knudsen number is from 0.072 to 7.23, which is dependent on the inlet pressure. The pressure is a constant, and the groove depth is reduced in the outlet region. The groove depth is taken as the characteristic length, and the Knudsen number is equal to 1.06 in the outlet region.

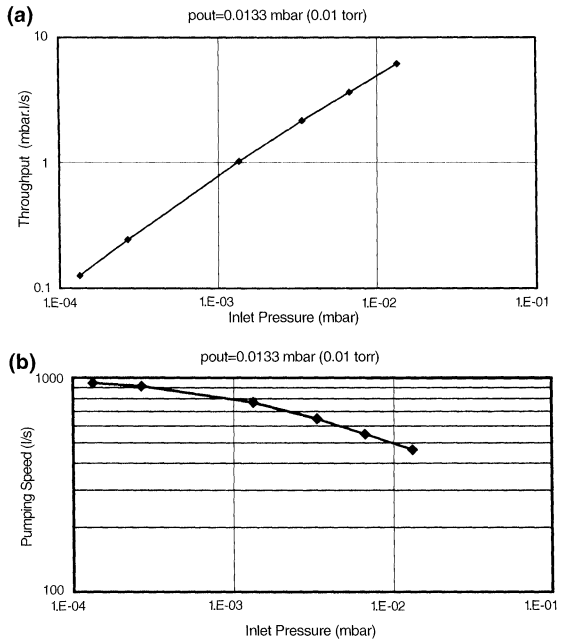

FIGURE 9 Throughput and pumping speed from DSMC numerical simulation.

5 CONCLUSION AND DISCUSSION

In this study, the Plücker coordinates are used to formulate the ruled surface wall and examine the molecules hitting the wall. It has succeeded in reducing the complexity of the algebraic geometry and computation. On the basis of analytic geometry, the intersection of the molecular path and ruled surface is found by the analytic solution of line geometry. The numerical simulation and experiment are shown in this paper. The result shows a reliable numerical simulation. If the flow field is surrounded by a ruled surface, the Plücker coordinates representation contributes an efficient tool in the DSMC method.

It is essential to establish a performance measurement system to evaluate vacuum pump performances and verify the numerical simulation result. The pumping speed measurement apparatuses and procedures are based on the industrial standard JVIS 005. A dry vacuum pump, Kashiyama SD 90V III, is chosen to be the foreline pump. The pumping speed experiment result is shown as Fig. 10.

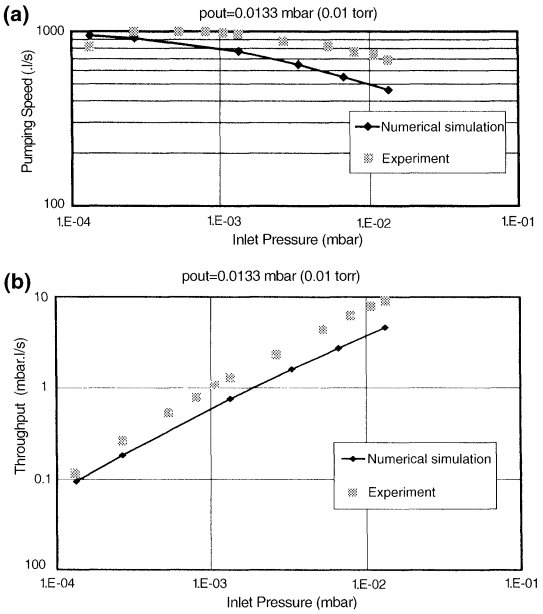

FIGURE 10 Pumping speed measurement result.

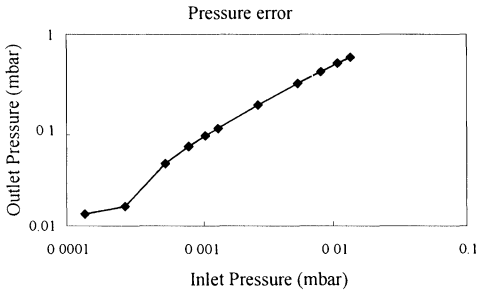

FIGURE 11 Outlet pressure error for boundary condition in numerical simulation.

In high vacuum, the numerical simulation is quite reliable. In the comparison of numerical simulation and experiment data, error exists in the rough and middle vacuum regime. The error from simulation due to the idealized boundary condition, which let the outlet pressure be a constant. The reality is that the outlet pressure is varied by the flow rate. The relationship between pumping speed and inlet pressure is an essential pumping characteristic of a foreline pump. The outlet pressure of a high vacuum pump is the inlet pressure of a foreline pump. The pressure error of boundary condition is shown in Fig. 11. The reference pressure is taken from the experiment. The pressure error is one of the reasons that contribute to the simulation error. If the real outlet pressure is considered in the simulation program, the numerical simulation is much closer to the experiment result.

The Plücker coordinates representation is not only applied to the analysis of this kind of molecular pump, but can also be applied to any other apparatuses with ruled surfaces. Excepting the work done in this study, future work will be focused on the development of the design criteria, such as optimizing the pumping performance at a specific pressure range.

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NOMENCLATURE

c	molecular speed of class c
$\vec{c}$	molecular velocity
D	characteristic length
f	velocity distribution of molecules
$\vec{F}$	force vector
Kn	Knudsen number
L, M, N, P, Q, R	elements of the Plücker coordinates
l, ϑ	a straight line
n	number density of molecules
$\vec{n}$	surface normal
$\vec{r}$	position vector
r_h	radius of rotor diameter

$\mathbf{r}(u)$	directrix
$\mathbf{v}(u)$	ruling vector
$\mathbf{r}(u, t)$	ruled surface with parametric form
$\mathbf{S}(u)$	ruled surface with Plücker coordinates
t	parameter; time
u	parameter of surface
z	length along axial direction
α	helix angle
λ	mean free path
Ω	solid angle of collision
θ	angle; rotational angle
$\bar{\theta}$	angle at initial position
σ	cross-section area

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