Analysis of the Compression Characteristics of Vapor Jet Injected into High Vacuum

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The working principle of diffusion pump, a kind of vacuum pumps, is to use the high momentum of vapor jet which is injected into high vacuum. Since flow regime inside the diffusion pump consists of continuum, transition and free molecular, a continuum approach is not valid to calculate the flow field. In this paper, the compression characteristics of a vapor jet into high vacuum were simulated using the direct simulation Monte Carlo (DSMC) method. The hard sphere model is used as a molecular model and the no time counter (NTC) scheme is employed as a collision sampling technique. Steady state flow characteristics such as velocity, temperature, density distributions of the pumped gas and oil vapor are calculated by simulating about hundreds of thousand molecules.

The main result is that the pumping speed of a single stage pump can be described based on the transmission probabilities which have nearly constant values irrespective of pressures at the inlet and outlet. Using these features, compression characteristics of diffusion pump can also be described by transmission probability concept as in the case of other high vacuum pump.

Key Words: Diffusion Pump, Transition Flow, Monte Carlo Method, Transmission Probability

Nomenclature

a, b	: Coefficients defined in Eq. (8)
A_a	: Area of the jet intake annulus $\pi(R_0^2 - R_i^2)$
C_U, C_U	: Aperture conductances based on the areas of the jet inlet and outlet annulus
Δt_m	: Discrete time step for molecular movement and collision in DSMC
g	: Relative velocity between molecules
l_s	: Nozzle length (see Fig. 2)
M	: Molecular weight
N	: The number of molecules in a cell
N_c	: Total number of collision pairs to be sampled in a cell
n	: Molecular number density
p	: Collision probability for each collision pair
P_U, P_L	: Gas pressures at the jet inlet and outlet in a single stage pump
Q	: Gas throughput
R	: Specific gas constant
R_i	: Radius of the boiler tube in a model diffusion pump
r, z	: Molecular position after movement in Δt_m and transformation
r^+, z^+	: Molecular position after movement in Δt_m and transformation
t	: Nozzle opening at the throat
T_{rU}, T_{rL}	: Transmission probabilities for forward and backward flow of pumped gas based on the jet intake annulus A_a
$\bar{v}$	: Mean thermal velocity

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$v(i), v^+(i)$: I-directional velocity components before and after movement in Δ_{tm}
w_P : Pumping probability

Greek Letters

β : Coefficient defined in Eq. (1)
γ : Ratio of specific heats
ρ : Density
θ : Angle between the boiler tube and the nozzle (see Fig. 2)
σ : Total collision cross section

1. Introduction

A variety of principles are used in modern vacuum pumping technology, and one of the most important mechanisms in high vacuum technology is the pumping by momentum transfer, where the momentums of the gas molecules to be pumped out are increased by collisions with a medium of high momentum, to a level high enough to maintain a steady flow against the pressure difference between a high vacuum pressure and the atmospheric pressure. Oil diffusion pump is one of the momentum transfer type pump, where the pumping action comes from momentum transfer by collisions between oil vapors of high momentum and pumped gas molecules.

Although the diffusion pump has been the most widely used pump for more than half a century with a variety of merits such as low price, no moving part, and constant pumping speed for all gases, design theories for diffusion pump are still at a very primitive stage, and most of the design and developmental works rely on primary principles coupled with experiments. The biggest problem with diffusion pump would be the prevention of oil vapor backstreaming, but the only solution available now would be the adoption of cold caps or baffles.

The key to the theory of diffusion pumping, either for improving the pumping performance or for reducing the oil backstreaming, lies in understanding the details of the collisions between oil vapors and gas molecules, which occur in the transition flow (not continuum, nor molecular) regime. That is why a quantitative analytical theory has remained undeveloped for very long. Reliable design theories are necessary in optimizing designs for different critical operating conditions and sizes, especially for designing diffusion pumps appropriate for UHV (ultra high vacuum) use.

Very recently the supercomputers opened a way to the solution of flow phenomena in the transition regime, and solutions for simple flows have been reported. Now it becomes possible to get theoretical solutions for the flow field and particle collisions in diffusion pumps, check the validity of old models, or develop a new realistic model.

Most of the early theories are for estimating pumping speeds for different gases. Even though real diffusion pumps have multiple stages, all the theories of diffusion pumps have been developed largely based on the simplified single stage configuration, which looks reasonable in the stable operation regimes.

One of the earliest models for diffusion pump is the pumping speed model proposed by Gaede and Matricon (Blears and Hill, 1948)

$$S=A(RT/2\pi M)^{\frac{1}{2}}[C-\beta(P_2/P_1)] \quad (1)$$

where A is the area of the jet annulus, and P_2/P_1 the pressure ratio across the pumping stage. The first bracket is the molecular incidence rate divided by gas number density on the jet opening. C is "the entrainment coefficient" representing the pumping probability, and β is the coefficient representing the back-diffusion of molecules from the forevacuum side to the high vacuum side. These two coefficients were thought to depend on the pump design and partly on the properties of the pumped gas, and have been determined by experimental methods.

Florescu (1960) proposed quite a realistic theory with the gas kinetic theory. Although the vapor flow was assumed to be one-dimensional with constant properties, the transport of pumped gas was considered to be a simplified diffusion process which is based on collisional exchange of momentum and energy at averaged velocities.

Toth (1968, 1982) refined the previous theories in several respects. Although the vapor flow was again assumed one-dimensional with prescribed velocity and density distribution, the interaction between the vapor and gas molecules was handled in terms of the Boltzmann equation which was solved by the simplified method of Chapman -Enskog. The resultant pumping characteristics could explain many of the thermogasdynamic effects in real pumps, but only qualitatively. Later, he extended his theory to the two-dimensional case, but stopped at the level of general formulation, without any solution.

Very recently, Rebrov and colleagues (Rebrov, 1986 ; Bulgakov et al. , 1988 ; Rebrov, 1990 and 1993 ; Iliasova et al. , 1993 ; Bulgakov, 1993) performed a series of design computations, but they computed the vapor flow field by solving the Navier-Stokes equation for vapor flow alone assuming the vapor flow to be a continuum unaffected by the gas molecules, then the pumped gas trajectories were computed by Monte Carlo method.

As is shown previously, most of the current theories of diffusion pumping rely on the one -dimensional models of the vapor flow, decoupling between vapor and gas flow, and also a few simplifying assumptions about the properties of vapor/gas molecules and the boundary conditions. There is only one exception of Iliasova et al. (1993), who considered the 2-D and 3-D distribution of flow parameters in the vapor-gas flow field, but here again the vapor flow was assumed to be a continuum and the interaction between vapor and pumped gas was not considered in calculating the vapor flow.

The pumping performance of diffusion pumps is determined by the structure of the oil vapor jet and the characteristics of collisions between vapor and gas molecules. Considering the theories and experimental results in previous researches, it is clear that the vapor jet expands to a very low density and is disturbed considerably by gas molecules in the vicinity of the jet boundary. Then it is unreasonable to consider the vapor jet flow to be one-dimensional. Also the one -dimensional theory can not explain the back diffusion of oil vapor which is very important in calculating the ultimate pressure.

Therefore, in this study, the complicated flow fields of oil vapors and gas molecules in diffusion pumps are precisely analyzed where no rigid assumptions on flow field or boundary condition are involved, and also the interaction between the vapor and gas molecules are simultaneously considered. Since the jet consists of two species (vapor and gas), the flow is in transition regime, and the geometry is complex, the only solution technique valid in solving the Boltzmann equation is the direct simulation method such as the direct simulation Monte Carlo(DSMC) method.

2. Theoretical Background

2.1 Pumping mechanism of the diffusion pump

In a conventional design of a diffusion pump (Fig. 1), the oil vapor as a pumping medium is produced in the heated boiler B by evaporation. It moves through an axisymmetric slit nozzle A, expands to a supersonic velocity, and finally becomes condensed on arriving at the pump wall C which is kept at a low temperature by a cooling

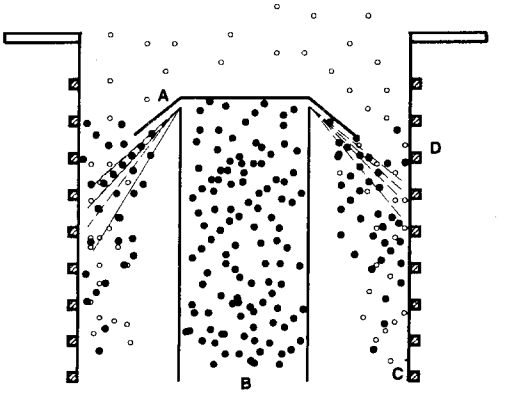


Fig. 1 Schematics of a single-stage diffusion pump model

water/air D. On their way from the nozzle throat to the wall, the vapor molecules make collisions with gas molecules, imparting some momentum to gas molecules.

Gas molecules, entering through the pump inlet, penetrate into the jet of the oil vapors and are given a downward momentum by collisions with oil vapors. The vapor jet normally flows with supersonic velocities. The gas-vapor mixture travels downward and radially outward, and only the oil vapors become condensed and return to the boiler in the liquid form by gravity when they strike the cooled wall of the pump body. The entrained gas molecules continue their path toward the next stage, and are finally removed by a mechanical forepump.

Without the vapor jet action, the diffusion pump is just an open channel, so the direction of the gas flow is determined by the relative pressures at the inlet and outlet. In vacuum pump system, the pressure at the outlet is usually higher, so a backflow is induced without the jet action. When the vapor jet is stably acting, the gas molecules penetrating backward from the outlet are struck back by collisions with vapor molecules, but the gas molecules entering through the inlet experience little resistance from the vapor molecules and even acquire extra momentum toward the outlet. So a stable gas flow can be maintained even when the exit pressure is much higher. This phenomenon can be explained in terms of transmission probabilities as follows.

For the gas molecules entering the jet through the inlet, the collision with vapor molecules always induces a sort of beaming effect, resulting in an increased transmission probability than without the jet action. But for the backstreaming gas molecules entering the jet through the pump exit, the collision with vapor molecules will have an effect of reversing the velocity direction toward the pump exit, resulting in a decreased transmission probability.

As the gas molecules from the inlet approach the outlet, they make frequent collisions with other gas molecules, through which their directional flow velocity become randomized and converted into an increased pressure. This is a sort of compression process, and is similar to the case of conventional centrifugal pumps or fans.

The supersonic vapor jet makes a very sharp turn at the edge of the nozzle cap, and some of the vapor molecules are struck into the upstream high vacuum space by collisions with high velocity gas molecules. These two effects induce the vapor backstreaming. When the gas density in the jet is high, the collisions between the gas and vapor molecules affect the motion of vapor molecules on a macroscopic level. Then the jet structure becomes altered by the gas flow.

The performance of a diffusion pump is dependent on the efficiency of energy transfer through collisions between oil vapors and gas molecules, which is in turn dependent on the density and velocity field of the jet, and also on the molecular weight of the oil vapor. The distribution of velocity and density in the vapor jet is determined by the nozzle shape, pump body geometry, boiler pressure and the gas density distribution. If the jet is too dense, the gas penetration into the jet will not be effective, and if the jet is too rarefied, the number of collisions for each gas molecule will be small. Both extremes will produce ineffective energy transfer, and an optimum value of density is required. The experimentally determined optimum boiler pressure is typically 1 to 2 torr. At this boiler pressure the vapor stream is not in the molecular flow condition but is rarefied enough to permit pumped gas molecules to enter deep into the jet. Then the vapor flow is in the continuum regime near the nozzle exit, but changes to the transition flow with further expansion.

2.2 Performance characteristics in terms of transmission probabilities

For general pumps and fans, the characteristic curve is expressed in terms of pressure rise versus flow rate, and the same is true of diffusion pumps except that the pressure rise is replaced by the pressure ratio, the compression ratio. This is because the pressure increases over several orders of magnitude in high vacuum pumps. And it is customary to express the flow rate (pumping speed) as a function of the pressure ratio (compression ratio).

Even though the primary variable in vacuum pumping is the pumping speed S or throughput Q, it is sometimes more convenient to formulate in terms of the pumping probability. In diffusion pumps, the jet structure and the pumping capability of the jet is not uniform. In this case, the pumping probability would be more appropriate than the pumping speed because the pumping probability can be defined as a spatially varying function while the pumping speed is only an average performance index. It is also possible to differentiate the pumping probability into two transmission probabilities in the flow and the reverse directions.

This kind of an approach is very useful because the distribution of transmission probabilities will be fixed once the jet structure is given. When the jet structure is unaffected by the gas flow or the pressures at the inlet and outlet, the transmission probabilities are fixed and the pumping speed for different pressures can be easily calculated. Pumping speed S can be written in terms of the pumping probability w_P as

$$S = C_0 \cdot w_P \tag{2}$$

where C_0 is the aperture conductance based on the area of pump inlet. When the pressure distribution is uniform both at the inlet and the outlet, pumping speed can be written in terms of the transmission probabilities in each direction as,

$$S = (C_U P_U Tr_U - C_L P_L Tr_L)/P_U = C_U Tr_U - C_L Tr_L\left(P_L/P_U\right) \tag{3}$$

where C_U and C_L are the aperture conductances based on the areas of the jet inlet and outlet annulus, P_U and P_L the gas pressures at the jet inlet and outlet, Tr_U and Tr_L the transmission probabilities for the pumped gas in the flow and the reverse directions based on the area of jet inlet and outlet annulus. Then the pumping speed can be calculated if only the transmission probabilities of pumped gas in each direction are given in terms of the operational conditions.

Most generally the transmission probabilities themselves are functions of the pressure ratio, because the jet structure and the resultary pumping action are dependent on the pressure ratio.

3. Simulation Techniques

3.1 Direct simulation monte carlo method

The flow in diffusion pumps is a complex nonequilibrium flow consisting of continuum, transition, and free molecular flow. This kind of flows can only be described by the Boltzmann equation, and various methods of solving the nonlinear Boltzmann equation exist, among which the direct simulation Monte Carlo (DSMC) method developed by Bird (1976) is one of the most widely used techniques.

According to this method, the motion of a very large number of molecules in a real gas flow is simulated through a much smaller set of representative simulation molecules. The paths of these simulation molecules are traced out in a physical space by a repetition of straight movements plus collisions with other molecules or wall surface for a small time interval Δtm. A computational grid cell system is generated in the physical space for selecting collision pairs and sampling flow properties. Each simulated molecule has three velocity components, three spatial coordinates, and species index. The number of collisions and collision pair selection in each cell are calculated in a statistical manner using the gas kinetic theory.

In this process, a scheme of generating random numbers and models for the molecular interaction are needed to sample the collision partners and to calculate the post-collision velocity. The macroscopic flow properties such as temperature and pressure can be obtained by sampling the molecular velocity in each cell. Reviews of the current status of this method can be referred to Bird (1978) and Muntz (1989).

In the present study, the NTC (No Time Counter) collision scheme developed by Bird (Boyd, 1991) is used to vectorize the collision calculation. In the NTC method, the total number of collision pairs to be sampled in each cell, N_c, is given by

$$N_c = \frac{1}{2} N n (\sigma g)_{\max} \Delta t_m \tag{4}$$

where N is the number of molecules in the cell,

n molecular number density, σ the total collision cross section, and g the relative velocity. When two particles in the cell are randomly selected, the probability of these two molecules making a collision is given by

$$p=\sigma g/(\sigma g)_{\max} \tag{5}$$

As a model for the molecular interaction in calculating the collision cross section σ and other collisional quantities, the hard sphere model was employed. While the size of pumped gas molecules is well known, the size of oil molecule is not readily available in most cases. In such a case, a spherical equivalent diameter, d, was calculated from the molar volume in the liquid state, molecular weight, and liquid density,

$$d=[(6M/\rho_L)/2\pi N_{AV}]^{1/3} \tag{6}$$

where M is the molecular weight, ρ_L the liquid density, and N_{AV} the Avogadro's number. The factor of 2 in the denominator is an approximate value accounting for the vacancy population of the liquid. In this study 546 g/mole and 1. 095 g/cm3 were used for N and ρ_L which are typical values of DC 705 oil.

The temperature considered in this study is translational kinetic temperature T_{tr} defined by

$$\frac{3}{2}\kappa T_{tr}=\frac{1}{2}m(\overline{u'^2}+\overline{v'^2}+\overline{w'^2}) \tag{7}$$

where m is the mass of molecule, κ the Boltzmann constant, and u', v', w' thermal velocity in each direction.

To assure accurate results in DSMC calculations, the number of simulated molecules should be as large as possible, the cell size much smaller than the mean free path, and the discrete time step Δt_m as small as possible in comparison with the mean collision time. In most of the calculations of this study, the cell size was smaller than the local mean free path except near the nozzle throat, and the discrete time step Δt_m was smaller than the mean collision time calculated at the nozzle throat condition.

When a molecule moves from a position (r, z) for time Δt_m, the new position (r^+, z^+) and new velocity $(v(1)^+, v(2)^+, v(3)^+)$ of the molecule are computed through the following transformation where the axisymmetry characteristic was made use of

$$z^+=z+v(3)\Delta t_m \tag{8}$$

$$r^+=[(r+v(1)\Delta t_m)^2+(v(2)\Delta t_m)^2]^{1/2} \tag{9}$$

$$v^+(1)=[v(1)(r+v(1)\Delta t_m)+v(2)^2\Delta t_m]/r^+ \tag{10}$$

$$v^+(2)=[-v(1)v(2)\Delta t_m+v(2)(r+v(1)\Delta t_m)]/r^+ \tag{11}$$

$$v^+(3)=v(3) \tag{12}$$

This transformation makes the calculation of boundary interaction very easy because all the molecules start to move from a same reference plane.

3.2 Pump models and boundary conditions

An axisymmetric slit nozzle in a cylindrical pump body was used as a model for a unit single stage pump (Fig. 2). The computational domain is defined by a number of point cells, and the areas for each cell are calculated by the Monte Carlo technique using the positions of the eight points surrounding the cell. In the figure, t is the slit height, ls the length of the nozzle, R_i the radius of boiler tube, P_U the inlet pressure, P_L the outlet pressure, and θ the nozzle angle. The height of computational domain H is fixed at 25cm and the nozzle angle $\theta=45°$, and t=1mm, unless mentioned otherwise.

The gas flow entering the open boundaries of the computational domain (nozzle throat, upper

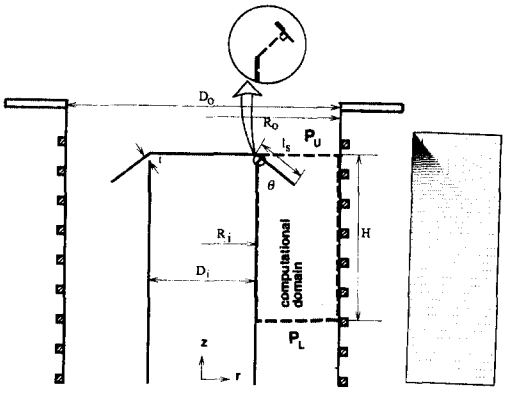


Fig. 2 Schematics of a simplified model for analysis and a cell system for a single stage diffusion pump.

inlet, and lower outlet) are assumed to be an equilibrium flow. The number of simulated molecules entering through each open boundary during a time interval and the velocity components of these molecules can be easily evaluated from the Maxwell distribution function if local pressure, temperature, and bulk velocity are known (Bird 1976). In this paper, sonic conditions are assumed at the nozzle throat, and the parameters at the throat were calculated from the one dimensional isentropic relations with stagnation pressure P_0 and temperature T_0:

$$T/T_0=\left(1+\frac{\gamma-1}{2}M^2\right)^{-1} \tag{13}$$

$$P/P_0=\left(1+\frac{\gamma-1}{2}M^2\right)^{-\gamma/(\gamma-1)} \tag{14}$$

where γ is the specific heat ratio of the oil vapor and M Mach number ($M=1$ at the throat). It was also assumed that the bulk velocity at the throat was uniform and in the direction of the equiangular axis of the nozzle. Gas molecules which enter through the upper and lower computational boundaries were assumed to have zero bulk velocity at pressures P_U and P_L respectively, and the velocities of these molecules (thermal velocity) are generated using the Boltzmann distribution.

Nominal values used in calculation are summarized in Table 1, where DC 705 was taken as the oil vapor and standard air for the pumped gas. All gas molecules striking the wall are assumed to be diffusely reflected with full thermal accommodation, and oil vapor molecules are considered to be perfectly condensed on the pump body.

The number of simulated molecules is in the range of $1\times10^5\sim2\times10^5$, and the number of computational cells is in the range of $2\times10^3\sim4\times10^3$. CRAY Y-MP C90/16512 was used and about 4 hours (in cpu time) were needed to attain a steady state for a given set of parameters.

In the process of simulation, the molecules are continuously moved into the computational domain through the open boundaries (nozzle throat, pump inlet and outlet) according to the boundary conditions, and the flow field is allowed to develop with time. The criterion for the attainment of a steady state is crucial in every steady-state simulation, and the criterion used in this study is that the relative difference between the total number of gas molecules entered, N_i, and the total number of gas molecules escaped, N_0, should be less than 0. 5% for each time interval.

$$\left|\frac{N_i-N_0}{N_i}\right|\leq0.005 \tag{15}$$

The time interval used in this criterion is the corresponding time needed for N_i to attain 30000.

The transmission probability Tr_U is defined as the ratio of the number of gas molecules which

Table 1 Parameter values used in the calculation

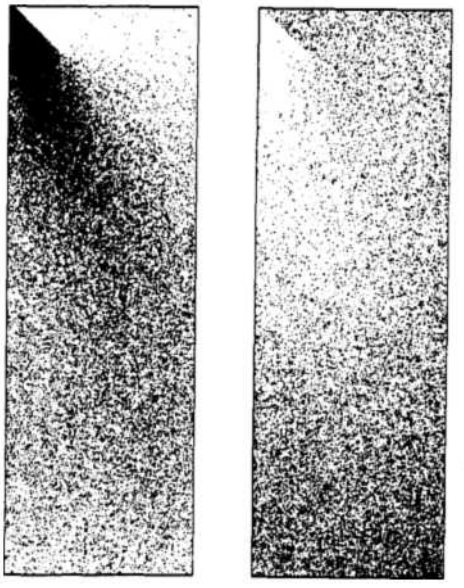
Parameter	Value
Stagnation vapor pressure P_0	1 mbar
Stagnation vapor temperature T_0	476 K
Diameter of the oil vapor molecule	$8.96\cdot10^{-10}$m
Diameter of the gas molecule	$3.64\cdot10^{-10}$m
Molecular weight of the oil vapor	497 g/mole
Molecular weight of the pumped gas	28.98 g/mole
Temperature of the pumped gas	300K
Specific heat ratio of the oil vapor	1.1
Temperature of the pump body	300K
Temperature of the boiler and the nozzle 476 K	

escaped through the lower computational boundary to the number of gas molecules entering through the upper computational domain. The transmission probability Tr_L can be defined similarly, if only the inlet and outlet are interchanged.

4. Results and Discussions

4.1 General flow characteristics in a model diffusion pump

When the simulation program is started, gas and vapor molecules begin to move into the computational domain through the open boundaries (pump inlet, pump outlet, and the nozzle throat), and the flow field develops with time. At first, the number of simulated molecules within the computational domain increases continually but comes to fluctuate about a certain level as the flow approaches the steady state. A typical instantaneous distribution of molecular densities for a single stage diffusion pump in the steady state is shown in Fig. 3. In this figure, dot points represent the positions of gas or vapor molecules. It is seen that gas molecules are rare in the core region of the vapor jet due to the frequent collisions encountered, and the gas molecules are gradually compressed along the pump body wall.



(a) Oil vapor molecules (b) Gas molecules

Fig. 3 An instantaneous distribution of molecular densities for a single stage diffusion pump in the steady state. ($R_0=13$ cm, $R_i=5$ cm, $l_s=3$cm, $P_U=10^{-3}$ mbar, $P_L=2\times10^{-3}$mbar)

Macroscopic flow properties in the steady state such as pressure, temperature, and velocity are shown in Fig. 4. As is predicted by the gas dynamic theory of nozzle expansion, the vapor flow emitting from the slit nozzle expands to a supersonic velocity, and the translational temperature of the vapor jet decreases with expansion. As the vapor molecules come to make collisions with gas molecules very soon, vapor temperature starts to increase. Even though the number density of vapor molecules is highest along the centerline of the nozzle, the isobars for vapor flow look like barrels with the boiler tube wall as their centerlines.

When the average gas pressure is low and the distance between the nozzle and the wall is large, the variation of vapor density is smooth and continuous. Therefore there is no rigid barrier for backstreaming gas flow, resulting in a low compression ratio (Fig. 4(a)). When the gas pressure is high and the nozzle is close to the wall, on the other hand, there is observed a sharp change or an increase in vapor density looking like a shock structure. Also a band of very high vapor density extends all across the flow aperture, which is a strong barrier against the backflow impling a very high compression ratio (Fig. 4(c)).

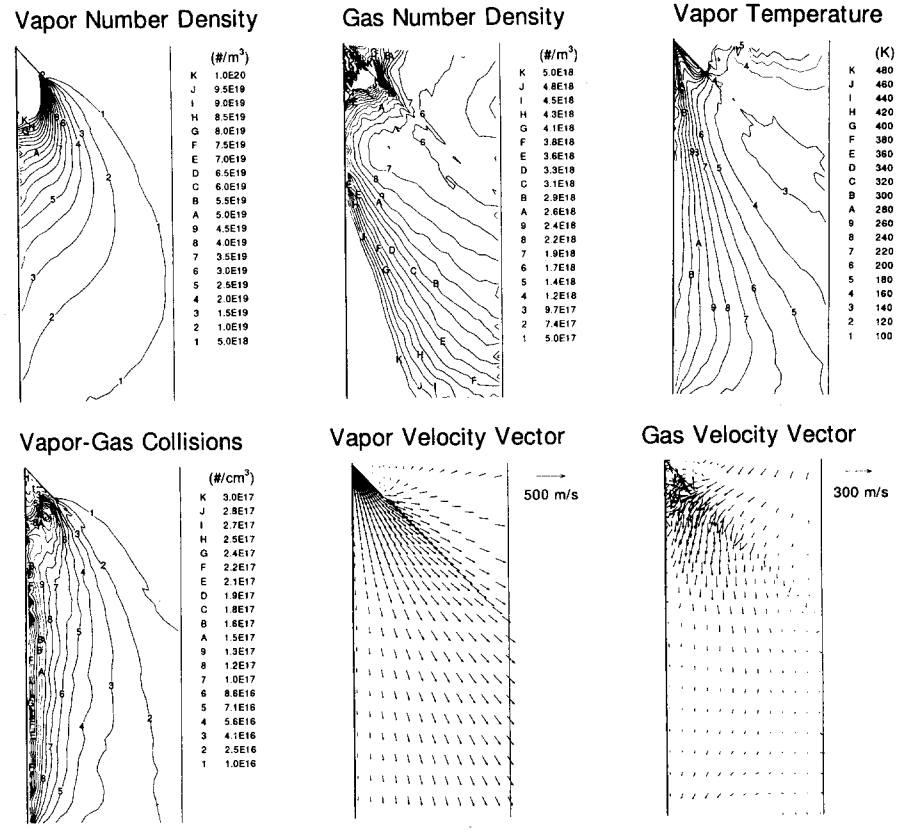
Some of the oil vapor molecules expanding along the inner suface of the top nozzle are struck by gas molecules or other vapor molecules to move toward the vacuum chamber. Since the backstreaming vapor molecules collide mostly on the gas molecules entering along the outer wall of the pump inlet, the bulk velocity of gas flow at the pump inlet gets decreased near the pump wall, and tends to incline inward to the nozzle side.

The gas molecules penetrating into the vapor jet are directed downward by the collisions made with vapor molecules, and become compressed gradually toward the exit due to the outer surface of the next nozzle or the high density gas molecules at the next stage. In general, the steady state gas pressure in the first stage domain is not higher than 3 to 4 times the inlet pressure unless the

vapor jet of the second stage becomes collapsed due to a high back pressure. Also bulk velocity of gas flow at the second stage inlet is quite small compared with the thermal velocity.

4.2 Pumping characteristics of a single stage pump

Even in a multi-stage pump, the vapor jets of different stages do not interact directly, but affect



(a) $R_t = 2$ cm, $P_U = 10^{-4}$ mbar, $P_L = 2 \times 10^{-4}$ mbar

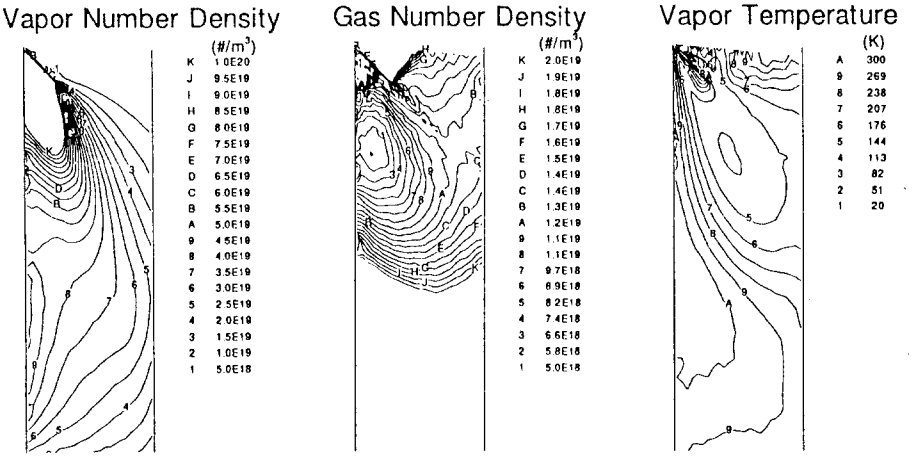
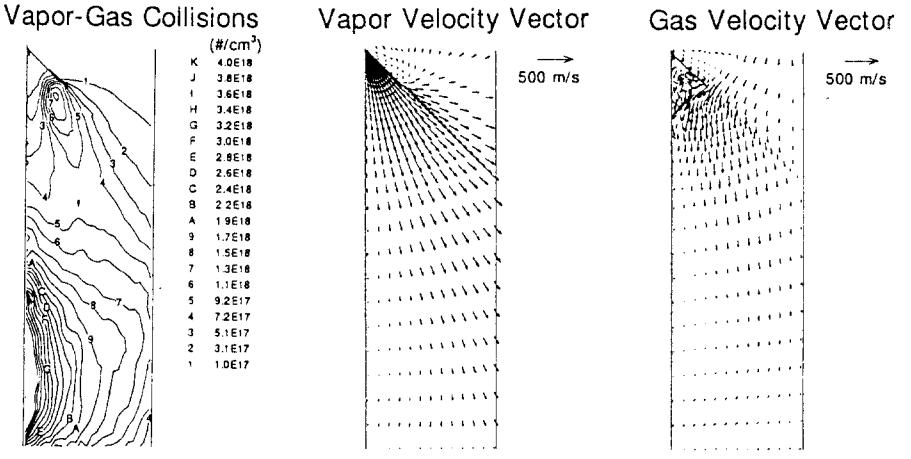
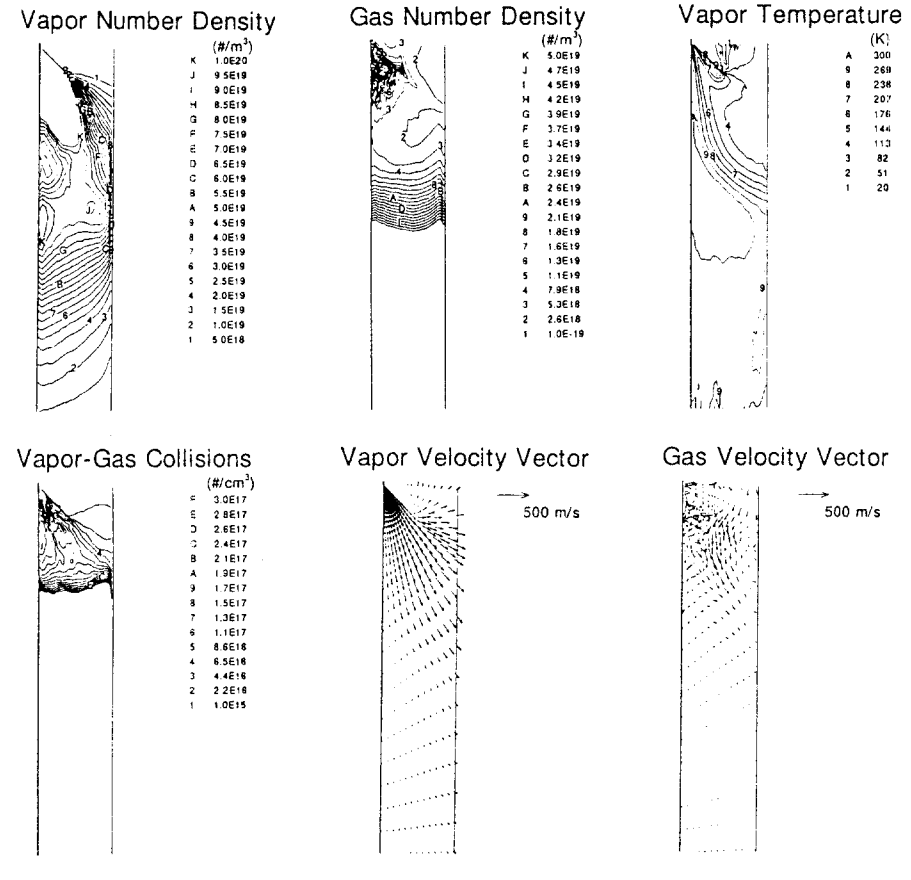


Fig. 4 (b) Continued



(b) $R_i = 5$cm, $P_U = 10^{-3}$mbar, $P_L = 2 \times 10^{-3}$ mbar



(c) $R_i = 8$ cm, $P_U = 10^{-4}$ mbar, $P_L = 5 \times 10^{-3}$ mbar

Fig. 4 Steady state flow characteristics of a single stage pump. (boiler wall and nozzle temperature = 300 K, $R_0 = 13$ cm, $l_s = 3$ cm)

each other through gas pressures. Then it is possible to separate a single stage, and its pumping characteristics investigated with boundary conditions imposed in terms of gas pressures. In a model single-stage pump, the exit is the whole annulus between the pump body and the boiler tube.

When the pumping action from the vapor jet is absent, the transmission probabilities in either direction is governed only by the solid boundaries, and are related as

$$C_i Tr_U = C_0 Tr_L \tag{16}$$

When the pumping action of the vapor jet comes into play, Tr_U usually becomes increased because the collisions have an effect of beaming the gas flow, but Tr_L becomes decreased because the collisions play the role of extra resistance to the reverse flow. When the vapor density is extremely high, even Tr_U can be reduced to some degree, but then the reduction in Tr_L would be much larger. So in any event the vapor jet induces a net forward flow from the pump inlet to the pump outlet. Results of direct simulation for a model pump with a small nozzle are shown in Fig. 5, and it is clearly seen that the vapor jet in the model pump increases Tr_U by about 15%, and decreases Tr_L to about 1/10 of the equilibrium value. The difference between Tr_U and Tr_L in the absence of vapor jet is caused by the nonuniform temperature distribution on solid boundaries.

The transmission probabilities in each direction for gas molecules are dependent on two factors. One is the jet structure which is determined by the collisions of vapor molecules making with other vapor molecules or gas molecules. The other is the collisions between gas molecules, but the gas-gas collisions are not so frequent in general, so can be neglected compared with other collisions. The vapor-gas collisions, however, can sometimes have an effect of altering the vapor jet structure. It means that the gas pressures at the inlet and/or outlet may change the jet structure, and so the transmission probabilities. Of the two pressures, the back pressure should have a much stronger impact on the jet structure because the collisions made with backstreaming gas molecules are much more than those with forward-streaming gas molecules. The effect of the back pressure on the jet structure would be dependent on the relative density ratio of the jet vapor to gas molecules. When the annulus for gas flow is large compared with the jet nozzle, the maximum expansion of the vapor jet is high, and the mean vapor density is low, then the jet is easily affected by the back pressure. When the annulus is small, the jet structure becomes more resistant to the back pressure because the vapor density in the jet is high.

For the model pump with a large nozzle, the transmission probability stays almost constant over a very wide range of back pressure, but for

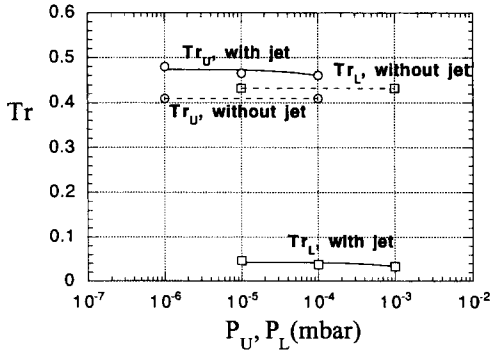


Fig. 5 Pumping effect of the vapor jet for a model single stage pump (R_0=15cm, R_i=5cm, l_s=4cm). The data on the dotted lines are for free molecular flow without oil vapor jet.

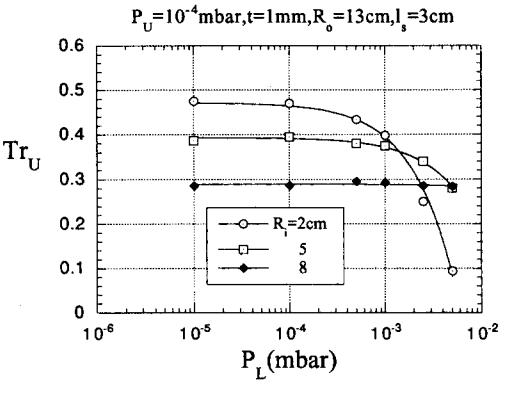


Fig. 6 Effect of the back pressure on the transmission probability of forward gas flow in a single stage pump.

small nozzles the transmission probability begins to decrease as the back pressure is increased over the chamber pressure (Fig. 6). In a conventional multi-stage diffusion pump, the nozzle of the second or the third stage has a larger size (R_i) than the first one in order to obtain a high compression ratio, and the maximum compression ratio in the first stage is at most 3 to 5. It follows that the forward transmission probabilities at each stage can be thought to be constant, irrespective of the back pressures of each stage, in normal operating condition. Then the analysis of forward and backward gas flow can be conducted independently for every stage. Furthermore, since the number of gas molecules is far smaller than the number of vapor molecules in most operational conditions, the transmission probabilities of forward and backward gas flow have nearly constant values irrespective of inlet or back pressure (Fig. 7).

As is shown above, the nozzle plays a decisive role in determining the pumping characteristics, and there are four parameters defining the nozzle geometry - radial position of the throat, size of the throat, the nozzle length, and the contour shape of the nozzle wall including the expansion angle. The determination of the nozzle length is important because it can also play a part in reducing the pumping speed. The calculated results show that a decrease in nozzle length does not always result in an increased pumping speed

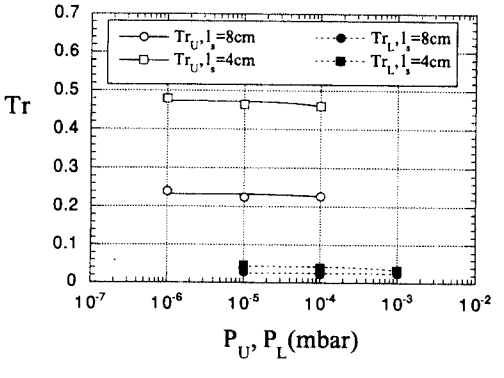


Fig. 7 Effect of the inlet pressure on Tr_U and the back pressure effect on Tr_L for a single stage pump (R_0=15cm, R_i=5cm).

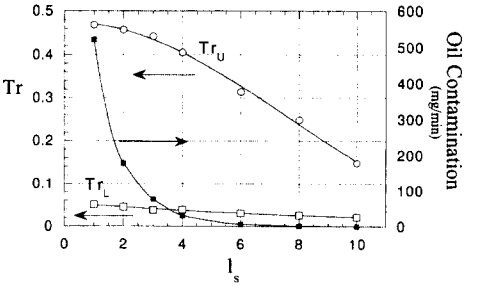
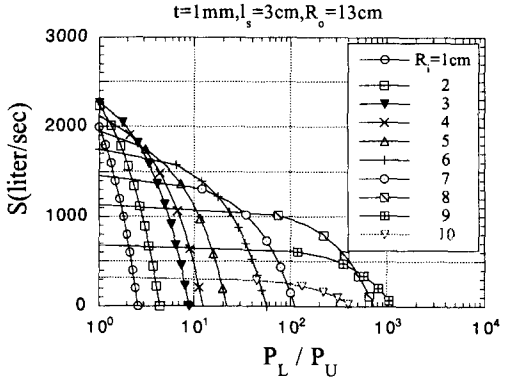


Fig. 8 Effect of the nozzle length on transmission probability and oil contamination for a single stage pump (t=1mm, R_0=13cm, R_i=3cm).

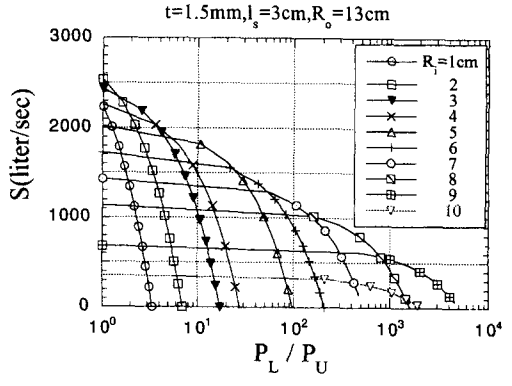
(Fig. 8). For long nozzle, the pumping speed increases as the nozzle length decreases, but if the nozzle becomes very short below a certain length, the pumping speed does not increase any more but stays unchanged, because the vapor density near the nozzle is too high for the gas molecules to penetrate easily. The transmission probability for the backward gas flow is almost insensitive to the nozzle length, because usual path for the backward flow is pushed toward the pump wall by collisions with vapor molecules. The oil contamination, which is defined by the number of oil molecules penetrating into the vacuum chamber through the pump inlet, decreases monotonically with the nozzle length.

As in Eq. (3), the pumping speed for a single stage pump is determined by the ratio of gas pressures at the pump inlet and outlet if the transmission probabilities for the pumped gas in the forward and reverse direction are known. Furthermore, the transmission probabilities are shown to have almost a constant value irrespective of inlet or back pressure, as illustrated in Fig. 6 and Fig. 7. Using these characteristics, the pumping speed for model single-stage pumps are calculated from the simulation data of the transmission probability. The area of pump inlet and the transmission probabilities for the forward and backward gas flow get smaller (the reduction in Tr_L is much larger than in Tr_U) as the nozzle size is increased either through R_i or l_s. For small nozzles, the maximum pumping speed which is obtained at zero compression ratio is high but

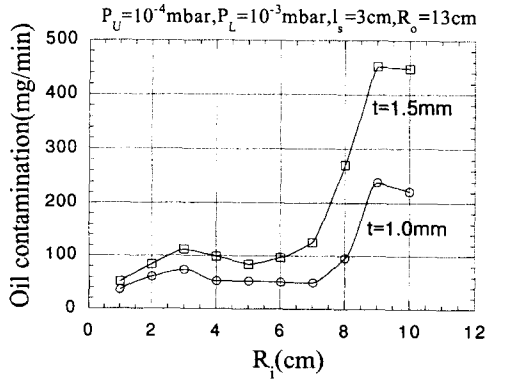
decreases very rapidly with compression ratio. On the other hand, for large nozzles, the maximum pumping speed is low, but stays almost constant over a wide range of compression ratios (Fig. 9 (a), (b)).



(a) Pumping speed for t=1 mm



(b) Pumping speed for t=1. 5 mm



(c) Oil contamination

Fig. 9 Pumping characteristics vs. nozzle parameters for a single stage pump.

If the size of the nozzle throat is increased, the mass flow rate of oil vapor is increased, and both the pumping speed and compression ratio increase with it, but a high oil contamination rate is also caused (Fig. 9(c)). In this figure, oil contamination was given in terms of the mass flux of oil vapors which escape through the upper computational boundary. This quantity has a tendency to increase with the nozzle throat area and also the flow annulus, and it has a large value when the nozzle size increases beyond the certain value because the nozzle does not cover all the region of high vapor density due to the high mass flow rate through the nozzle throat in this case.

5. Conclusions

The pumping characteristics of model diffusion pumps were simulated by the vectorized DSMC method. The hard sphere molecular model and No Time Counter collision scheme were adopted. Major conclusions from these analyses for model diffusion pumps can be summarized as follows:

(1) When the average gas pressure is low and the distance between the nozzle and the wall is wide, vapor density becomes smooth and continuous, but when the gas pressure is high and the nozzle is close to the wall, there is a sharp change of vapor density such as shock structure.

(2) The vapor jet helps the forward flow and hinders the backward flow. When compared with the case of no jet action, the probability of forward transmission is increased a little but that of the backward flow is decreased to a very low value. The change in flow probabilities is strongly dependent on the nozzle size, and moderately dependent on the size of nozzle throat. The effect of back pressure on the transmission probability getting larger as the nozzles become smaller, but under normal operational conditions of multi -stage pumps, the transmission probability at each stage can be thought to be nearly constant irrespective of the pressures at the pump inlet and outlet.

(3) In the first stage nozzle, there exists an optimum length in such a way that when the nozzle length becomes smaller than the optimum,

the pumping speed doesn't change but oil back-streaming increases sharply.

(4) The performance of multi-stage pumps can be analysed by combining the transmission probabilities of forward and backward gas flow for a single stage pump.

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