Pergamon

Vacuum/volume 46/numbers 8–10/pages 863 to 866/1995
Elsevier Science Ltd
Printed in Great Britain
0042–207X/95 $9.50+.00

0042-207X(95)00058-5

Numerical modelling of the molecular and transitional flow regimes in vacuum components

Godela Scherer-Abreu, *Department of Pure and Applied Mathematics, Simon Bolivar University, Apartado Postal 89000, Caracas, Venezuela*

and

Raul A Abreu, *Edwards High Vacuum International, Manor Royal, Crawley RH10 2LW, UK*

Based on the assumptions of the kinetic theory of gases, a three-dimensional probabilistic model of molecular and transitional flow in vacuum components was developed. The computational model takes as data combinations of pressures, temperature of the gas and of the container, type of gas, and geometry and type of materials used in the vacuum components. The results of the calculations are gasflow, dependent pressures and molecular density distribution. In order to treat complicated three-dimensional shapes effectively, an adaptive cell generation method was designed. The model was tested for several geometries with static and moving walls and different flow conditions, and was found to agree well with published results.

1. Introduction

The gas flow through a vacuum component can be continuous, transitional or molecular depending on the pressure range and geometries involved. A review of existing calculation methods in gas dynamics shows that attempts have been made to produce a numerical scheme able to treat the whole range from continuous to molecular flow[1]. But the available models are, for the time being, only applicable to inviscid, incompressible flows at the continuous end of the spectrum. This approach is not valid for the modelling of vacuum components and it is still necessary to solve the different flow regimes separately, with different methods. For continuous flow, a numerical solution of the full Navier–Stokes equations has to be considered. A recommended approach would be to use the implicit Beam-Warming scheme with an explicit treatment of the viscous term. For molecular and transitional flows, numerical methods for solving Boltzman's equation have been extensively studied[2]. For molecular flow, results have also been obtained through Monte Carlo simulations based directly on the molecular description provided by kinetic theory[3,4]. Several authors have worked on the extension of the simulations to transitional flow where intermolecular interactions have to be considered[2,5–7], but due to their unmanageable computing requirements they have been found feasible only for simple one-dimensional or axisymmetric problems. Even so, some results have been obtained only by using a parallel computer[7].

The present work proposes a method for simulating molecular and transitional flows using a probabilistic model in three dimensions. The result of the simulation is a molecular distribution function throughout the region. Once this function is obtained it is used to calculate variables such as density, pressure etc. The model was tested by calculating transmission probabilities, mass flow in tubes, and throughput for a simplified Gaede pump. The results of these numerical experiments were compared with values given in the literature and found to agree to within 5%. The present version of the software, written in FORTRAN, can be run on a 486DX microcomputer.

2. Modelling of molecular and transitional flow

A complete description of a fluid from a molecular viewpoint can be given by the molecular distribution function $f(\mathbf{r}, \mathbf{v}, t)$, which is a function of the position vector $\mathbf{r}$, the velocity vector $\mathbf{v}$ and time t. The quantity $f(\mathbf{r}, \mathbf{v}, t)\ \mathrm{d}\mathbf{r}\ \mathrm{d}\mathbf{v}$ is the mean number of molecules whose centre of mass at time t is located between $\mathbf{r}$ and $\mathbf{r}+\mathrm{d}\mathbf{r}$ and has a velocity between $\mathbf{v}$ and $\mathbf{v}+\mathrm{d}\mathbf{v}$. From the function $f(\mathbf{r}, \mathbf{v}, t)$, macroscopic quantities that describe a flow such as density, pressure, temperature and stream velocity can be deduced by averages of molecular values in a space element. The distribution function can be obtained through probabilistic simulations. In this work, a statistically representative set of particle histories is generated to obtain a good approximation to the distribution function. Intermolecular and molecule–wall collisions are considered in these histories.

Particles are assumed to enter the vacuum components from large containers in which the gas is Maxwellian. The inward number flux of molecules is proportional to the gas density and the average thermal speed of the molecules. The probability that a molecule enters an elementary area of an opening is proportional to this area and the probability that a molecule enters in an elementary solid angle is proportional to the cosine of the angle with respect to the normal to the surface (cosine law).

For the intermolecular collisions the following assumptions are made:

(i) Molecular chaos: possible correlations between pre-collision velocities of molecules can be neglected.
(ii) Only two-particle collisions are taken into account.
(iii) Molecules are perfectly elastic.
(iv) The hard sphere model is considered: intermolecular forces become effective at molecular diameter distance only and the deflection angle depends only on the eccentricity of the impact.

There remains only to analyse the molecular interactions with the walls. The wall collision dynamics are based on an assumption of Lorentz that the solid walls are 'molecularly rough' and therefore perfect diffusers[3]. The molecules striking the wall become adsorbed there for a time (residence time) and on leaving the wall have forgotten the incident direction and velocities. The behaviour of diffusely reflected molecules is identical to that of molecules from a fictitious equilibrium gas on the reverse side of the surface, therefore the cosine law again applies.

3. Numerical modelling

The computational model was designed for simulations of time dependent flows in a given physical space with static and moving boundaries. Simultaneous particle histories are generated. For each particle (a kind of macromolecule in lieu of a large number of real molecules), position vectors at the entrance wall, uniformly distributed over the surface, and velocity vectors with a direction distribution that is proportional to the cosine of the angle with the normal, are generated. If the entry plane is normal to the z axis, the initial direction of emission at point $(x, y, 0)$ with a cosine law probability is defined by the direction cosines (α, β, γ), where $\alpha = p\cos(\phi)$, $\beta = p\sin(\phi)$, and $\gamma = q$. Here p, q and ϕ are obtained from two numbers, r_1 and r_2, chosen from a uniform distribution in (0, 1) as follows: $p = \sqrt{r_1}$, $q = \sqrt{1-r_1}$, and $\phi = 2\pi r_2$.

The position and velocity vectors are updated in time, taking into consideration wall–molecule and molecule–molecule collisions. From these information vectors, an approximation to the molecular distribution function and the desired macroscopic variables are calculated.

A discretisation of time and space has to be defined. The time intervals $\mathrm{d}t$ are chosen small enough to be able to consider, separately, pure molecular motions without intermolecular interactions, followed by the appropriate molecular collisions. Therefore $\mathrm{d}t$ has to be smaller than the mean collision time (depending on the gas density). Action is taken if the molecules cross an exit boundary or hit a wall. Then the collisions occurring during $\mathrm{d}t$, among particles that are close enough (belonging to the same cell), are simulated.

Space is subdivided into a cell structure which follows the boundaries as closely as possible. First, the whole domain is covered by a set of points, each point associated with a norm, and acting as the identifier of an element of volume or cell. A molecule belongs to a cell if its position is close enough to the reference point in a given norm. The shapes of the cells can vary with the norm from simple cubic with

$$\|\mathbf{x}\|_\infty = \max_i |\mathbf{x}_i|$$

to more complicated curved forms when using modified Euclidean norms. The cell shape and size can therefore be adapted to more complicated geometries and regions of larger gradients. The boundaries could also be covered by points, and a wall hit would be identified as such if the molecule entered the one-sided small cell associated with a boundary point. The direction distribution of the velocity vector of the reflected particle is obtained by a rotation. The rotation matrix is formed using the angle between the normal to the surface at the boundary point and the z axis. The schematic flow chart is shown in Figure 1.

4. Results and discussion

To test the molecular flow 'aspect' of the program, the transmission probabilities of tubes of various shapes were calculated and the results compared with values taken from formulae found in the literature[8,9]. When calculating the transmission probability the following assumptions must be made: stationary flow conditions, constant flow current density at the entry plane, and molecular flow.

For long tubes of length l and rectangular cross-section $A = b \times a$, the equation for the transmission probability Pr given by Wutz *et al*[8] is

$$Pr = \frac{8}{3}\frac{b}{l}\frac{1}{1+\gamma}\frac{1}{\Phi_R(\gamma)} \tag{1}$$

where $\gamma = b/a < 1$, and $\Phi_R(\gamma)$ is a correction factor taken from a graph. This equation was evaluated for $A = 1$ cm^2 and $A = 0.1$ cm^2, and values of l/b between 1 and 100 with $l = 100$ cm. Pr values from equation (1) and the corresponding calculated transmission probabilities P_k are shown in Figure 2. The agreement is within 5%, even for long and narrow tubes ($l/b = 100$).

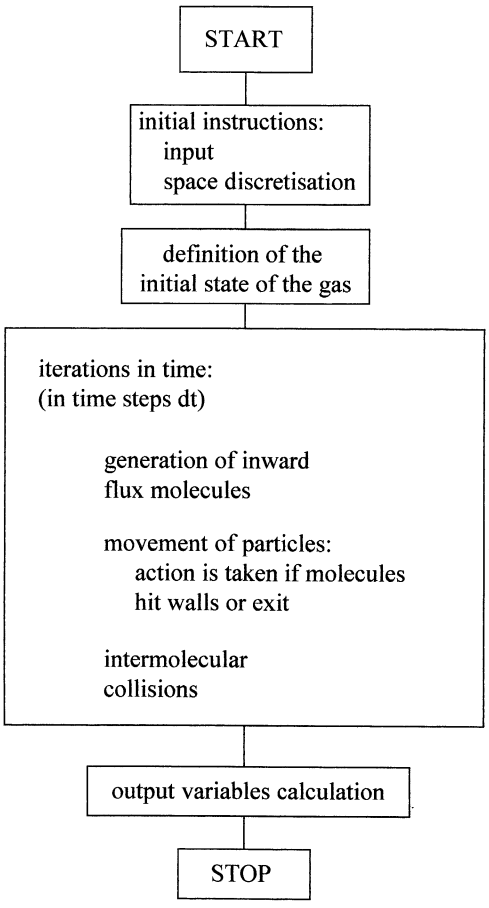

Figure 1. Flow chart of computational model.

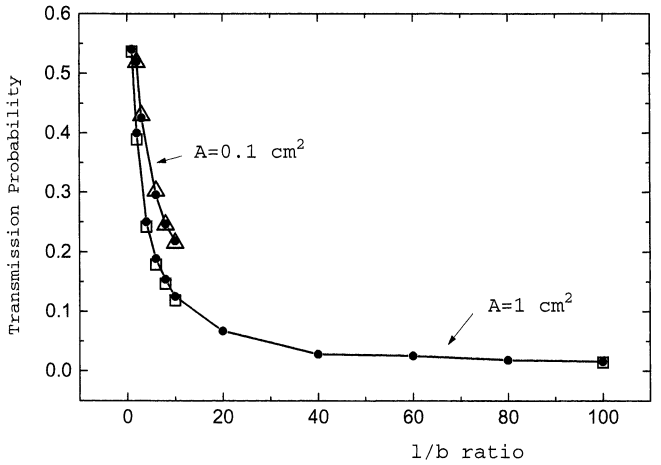

Figure 2. Transmission probability in tubes of length l and width b, with rectangular cross-sections $A = 0.1$ cm^2, and $A = 1$ cm^2, as a function of the l/b ratio. The circles joined by solid lines represent the data reported by Wutz *et al*[8], and the squares and triangles the results of the calculations.

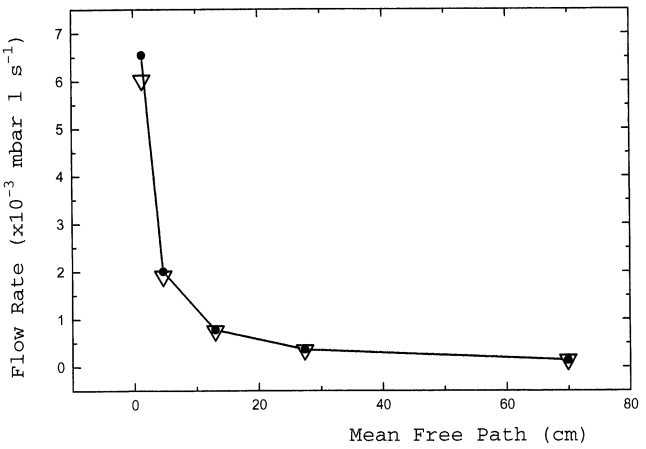

Figure 4. Flow rate as a function of the mean free path for a tube of rectangular cross-section. The circles joined by solid lines are the results of experiments by Dong and Bromley[10]. The triangles represent the calculated flow rates.

Figure 3 shows the transmission probability Pr reported by Clausing[9] for a tube of circular cross-section of radius r and length l, and the calculated transmission probability Pr. The agreement is better than 5% through the three decades of the l/r ratios.

The transitional and molecular aspects of the model were tested for the case of a tube of rectangular cross-section in which pressure and flow measurements were taken in molecular and transitional flow[10]. The dimensions of the tube were 0.324 cm wide, 22.86 cm high and 60.96 cm long. The two lower values of the mean free path (4.61 and 1.32 cm) are indicative of transitional flow in this geometry in which there is some molecular interaction. Figure 4 shows the measured flow rate Q and the calculated flow rate Q_k as a function of the mean free path calculated from the average pressure.

A simplified element of a Gaede type pump was modelled in order to test the program for moving boundaries. The compression ratio of the Gaede pump reported by Biank and Petzold[11] from the Mongodin and Prevot theory was taken for comparison. Consider parallel plates of side $a = 3.6934$ cm and length $L = 37.989$ cm separated a distance $h = 1.0553$ cm, and one of the plates moving at speed $u = 8300$ cm s^{-1}. The pumping speed S_k is expressed as

$$S_k = \frac{ahu}{2\times 10^3}\,\frac{e^{\alpha}-P_V/P_H}{e^{\alpha}-1} \qquad (2)$$

where P_V is the inlet pressure, P_H the exhaust pressure, P_V/P_H the compression ratio and

$$\alpha = \frac{uL}{h}\sqrt{\frac{M}{2\pi RT}}.$$

For a compression ratio of 18.89 the pumping speed calculated by equation (2) is $S_k = 11.5$ l s^{-1}; the value obtained with the numerical model was 12.6 l s^{-1}. This result demonstrates the potential use of the model in predicting the performance of molecular pumps.

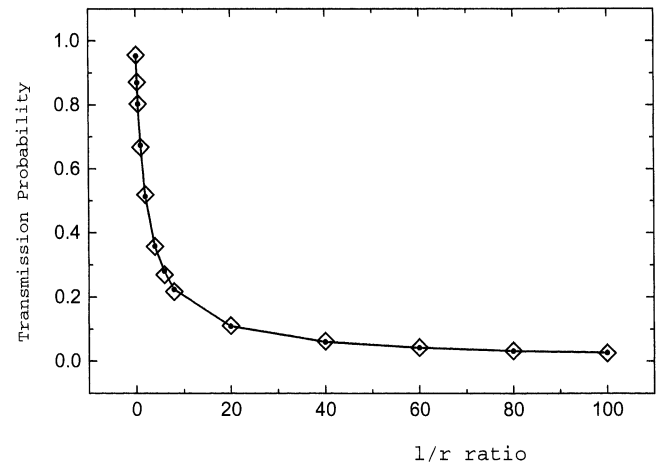

Figure 3. Transmission probability in tubes with circular cross-sections, radius r and length l, as a function of the l/r ratio. The circles joined by solid lines are the data reported by Clausing[9], and the diamonds are the results of the calculations.

5. Conclusions

We developed a three-dimensional numerical model to calculate flow in vacuum components based on a space discretisation scheme that can adapt to complex physical shapes with stationary or moving boundaries. The model was tested, and the results were compared with published data in molecular and transitional flows. It is not restricted to any particular geometry, and can be easily extended to treat any arbitrary shape automatically.

Acknowledgement

One of the authors (GS) would like to thank CESMA at Universidad Simon Bolivar, for the use of their computer facilities.

References

[1] F Coron and B Perthame, Numerical passage from kinetic to fluid equations, *SIAM J Numer Anal*, **28**(1), 26 (1991).
[2] G A Bird, *Molecular Gas Dynamics*, Clarendon Press, Oxford (1976).
[3] L Loeb, *The Kinetic Theory of Gases*, Mc Graw-Hill, New York (1934).
[4] D Davis, Monte Carlo calculations of molecular flow rates through a cylindrical elbow and pipes of other shapes, *J Appl Phys*, **31** (7), 1169 (1960).

[5] L Fustoss, Monte Carlo calculations for free and near free molecular flow through axially symmetric tubes, *Vacuum*, **31**(6), 243 (1981).
[6] J K Haviland, in *Methods of Computational Physics*, Vol 4, p. 109. Academic Press, New York (1985).
[7] Masahiro Ota and Hiroyoshi Taniguchi, Transmission probabilities of gas molecules through finite length tubes in transition ranges, *Vacuum*, **44**(5/7), 685 (1993).
[8] M Wutz, H Adam and W Walcher, *Theory and Practice of Vacuum Technology*, F. Vieweg (1989).
[9] P Clausing, The flow of highly rarefied gases through tubes of arbitrary length, *J Vacuum Sci Technol*, **5**(5), 636 (1975).
[10] W Dong and L A Bromley, Vacuum flow of gases through channels with circular, annular and rectangular cross-sections, *Trans 8th National Vacuum Symposium of the AVS*, Vol. 2, p 1116. Pergamon Press, Oxford (1961).
[11] H Biank and K Petzold, Zur Sauggeschwindigkeit der Molekularpumpe, *Vakuum-Technik*, **12** Jhrg. Heft 3, 82 (1963).