DEPARTMENT OF CHEMICAL SCIENCES
SCHOOL OF SCIENCES AND HEALTH PROFESSIONS
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NORFOLK, VIRGINIA

ANALYSIS OF FLOW DYNAMICS THROUGH
SMALL DIAMETER GAS SAMPLING SYSTEMS

By

Kenneth G. Brown, Principal Investigator

Final Report
For the period July 1, 1983 to January 1, 1984
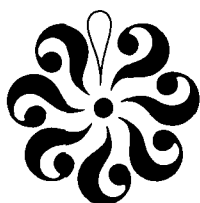
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OLD DOMINION UNIVERSITY RESEARCH FOUNDATION

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INTRODUCTION

The removal of gas material through a capillary opening in a surface is analyzed. The gas, from which the sample is removed, is moving past the surface at supersonic velocities. A variety of possible conditions of temperature, pressure and composition are discussed in an effort to emulate conditions that (1) might be found at the surface of a vehicle traversing the altitude range 100-50 km, or (2) possibly exist at the surface of a model in the stream of a high enthalpy wind tunnel. We will be concerned with determining (1) the throughput of the capillary for conditions of different lengths and different L/a (length/radius) ratios, (2) the total throughput when the surface in question contains many hundreds of these capillaries, (3) the effect of the capillaries upon the composition of the analyzed gas, (4) the effect of the capillary or capillaries upon the gas stream itself, and (5) the implications of the calculations upon the possible implementation of this type of device as an inlet for a mass spectrometer to be developed for analyzing the upper atmosphere.

MODEL PARAMETERS

As this capillary or assembly of capillaries is to be mounted at the surface of a reentry vehicle, it is necessary that the surface conditions as a function of altitude can be obtained either from experiment or calculation. The two most important parameters in determining the flow

*Associate Professor, Department of Chemical Sciences, Old Dominion University, Norfolk, Virginia 23508

characteristics are the temperature and pressure at the surface. The pressure at the surface of a reentry vehicle can be determined using a program developed by Shinn, Moss and Simmonds [1] assuming a shape for the model and a suitable flight path angle. These calculations have been performed by Eide [2] at altitudes of 55 km, 64km, 72 km and 84 km. The shape of the model was a combination of a sphere and cone to produce a blunt-nosed reentry vehicle. One point at the surface was selected for all of the calculations in this report. The dimensionless coordinates of this point are (.013, .017) (see ref. 1), a point slightly behind the point that represents the merger of the sphere and cone used to generate the shape of the model. The calculated wall values at this point for the above altitudes are given in table I.

Table I. Surface values for the parameters as a function of altitude.

Altitude	55 km	75 km	73 km	84 km
Pressure (atm)	.0686	.0339	.0151	.00405
Temperature (K)	1480	1620	1590	1560
density (g/cm)	$1.53 \ 10^{-5}$	$6.67 \ 10^{-6}$	$2.87 \ 10^{-6}$	$7.92 \ 10^{-7}$
viscosity (poise)	$5.59 \ 10^{-4}$	$5.93 \ 10^{-4}$	$5.94 \ 10^{-4}$	$5.9 \ 10^{-4}8V$

CALCULATION OF THE MEAN FREE PATH

To help determine whether the flow will be molecular, viscous, or transition, the mean free path for the various gases under consideration must be determined at each altitude. To estimate the mean free path the following equation developed by Sutherland [3] will be used:

$$\lambda = 8.589 \ (\eta/P) \ (T/M)^{\frac{1}{2}} \ cm \qquad (1)$$

where ̄ = mean free path

n = viscosity in poise

P = pressure in mm

T = temperature in K

M = molecular weight

The results of these calculations are shown in table II for O atoms, O_2, N_2 and CO_2. The largest mean free path (MFP) is for O atoms at 84 km

Table II. The mean free path of the various species. All values are calculated using equation (1). All values divided by 10^{-4} cm.

	55 km	65 km	73 km	84 km
O	8.86 km	19.9	44.3	162
O_2	6.26	14.1	31.3	11.5
N_2	6.7	15.0	33.5	123
CO_2	5.34	12.0	26.7	98

and is approximately 160 microns while at the lower altitudes the MFP drops to approximately 5 microns for CO_2. This variation in MFP would indicate that at a capillary radius of 10 microns the flow may be molecular at high altitudes with a $\lambda/a = 16$, with an increase in the viscous nature of the flow at lower altitude. It is more likely, however, that the bulk of the flow will be in the transition region where the flow will be neither molecular nor viscous. In order to determine the relative importance of these two types of flow the calculations will be performed assuming (1) that the flow is of either nature, and (2) a treatment of the flow that tries to simulate the transition (slip) region will be utilized. The results of these different calculations will then be compared.

3

VISCOUS FLOW

For the purposes of this report, it will be assumed that the viscous flow will be given by Poiseuille's equation corrected for length. This equation is given below:

$$Q = \frac{\pi a^4 P(P_2 - P_1)}{8\eta L \left(1 + 1.14 \frac{N}{8\pi\eta RT} \frac{Q}{L}\right)} \tag{2}$$

where a = radius of the capillary (cm)

L = length of the capillary (cm)

M = Molecular weight

P = pressure in microns

η = viscosity in poise

R = gas constant

Q = flow in micron-liters/sec.

N = Avogadro number

All viscosities are calculated using the equations and programs developed in reference 4. The exit side of the capillary will be maintained at a pressure of 10-5 torr, or less, so that P can be ignored. Dividing the above equation by the pressure yields the conductance, F, which has units of liters/second. The calculated flow for pure N_2, air, and CO_2 in air are compared in figure 1 as a function of inlet pressure for different L/a ratios. Since O_2 and CO_2 are minor constituents the viscosity does not change and the curves for the three cases overlay at the assumed temperature of 1500 K. (This temperature represents an average for the temperatures presented in table I. At a constant temperature and pressure there will not
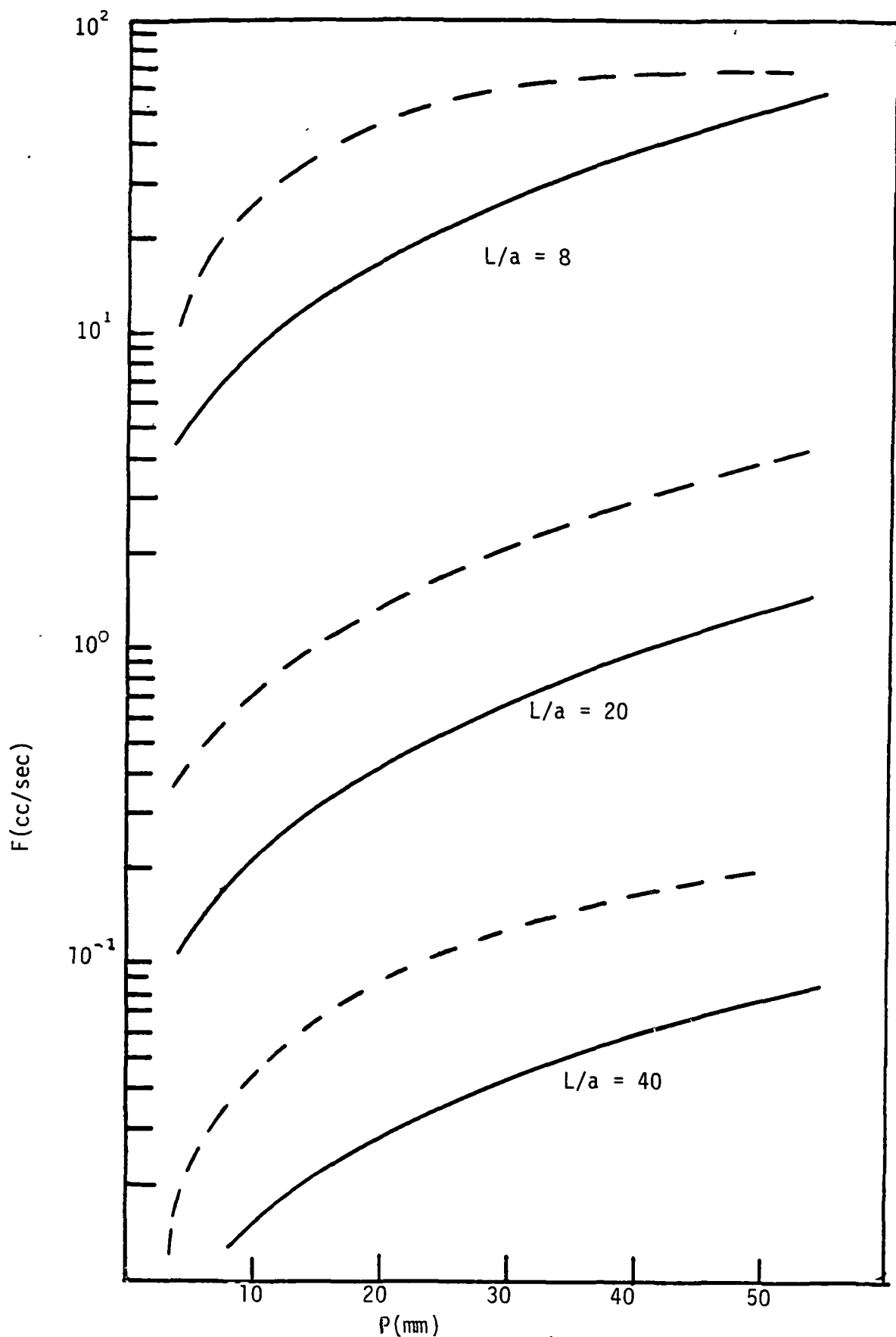
Figure 1. Viscous flow, as a function of pressure, for Nitrogen, Air, and Air-1% CO_2 at three different values of L/a. As the viscosities for all three are the same there is only one curve at each L/a. (-1500K, ... 300K)

be a capillary induced effect upon the composition of the removed gas for viscous flow.

MOLECULAR FLOW

If the MFP is greater than the characteristic dimension, in this case the radius, then the flow will be governed by collisions with the opening rather than with other molecules. In addition, if the length of the capillary is short enough the flow will remain molecular throughout the capillary. To calculate the flow the following formula developed by Clausing is used:

$$F = 3.638KA(T/M)^{\frac{1}{2}} \qquad (3)$$

where F is in liters/sec, A is the area of the orifice, and T and M are the temperature and molecular weight, respectively. K is a constant which corrects the flow for the length of the capillary. Values of K are quoted in standard reference books as a function of L/a. In the limit of large L/a (>1000)

$$K = 8a/3L . \qquad (4)$$

The calculated molecular flow rates for O atoms and N_2 are compared to the calculated viscous flow rates in figure 2, for a = 100 and 10 as a function of a/L. An immediate observation is that, if the flow is molecular, the observed flows through the capillary will have to be corrected for molecular weight. Also, for a very small radius capillary the flow will be greater in the molecular case than in the viscous case, at the pressures considered.
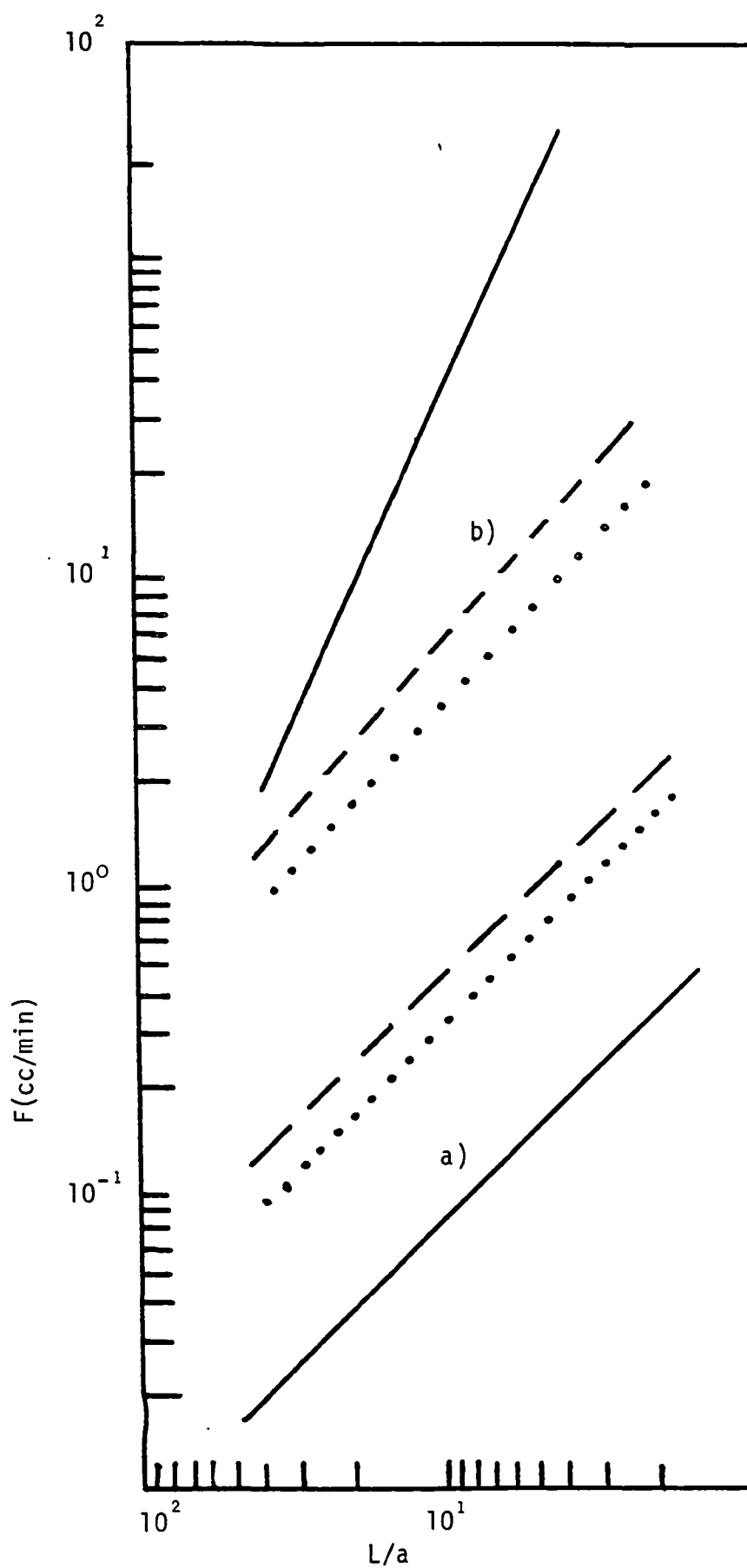
Figure 2. A comparison of calculated molecular flow for O atoms
(---) and N₂(...) with calculated viscous flow (-)
a) a = 10μ   b) a = 100μ.

COMBINED FLOW

The above calculations represent the two limiting cases for flow. It is necessary, however, to account for the possibility that the flow will be in the transition (slip) region. Knudsen [5] observed that as the pressure increases, the flow through the capillary actually reached a minimum value in the transition region. One possible model, which attempts to account for the transition region and combine molecular and viscous flow, was proposed by Scott and Dullien (6,7). They assumed that the fraction $G(a/\lambda)$ of the collisions with the walls which resulted in the particles being backscattered, not transmitted through the tube, or which occurred without an intermittent intermolecular collision is given by:

$$G(a/\lambda) = \frac{4}{\Pi} \int_{o}^{\frac{\Pi}{2}} \int_{o}^{\frac{\Pi}{2}} \sin\theta \cos\theta \ e^{-\left(\frac{\cos\theta}{\sin\theta}\right)\left(\frac{2a}{\lambda}\right)} d\theta \ d\phi. \quad (5)$$

An approximate solution for the above equation is:

$$\alpha(a/\lambda) = e^{\sinh\left(\frac{2a}{\lambda}\right)}. \quad (6)$$

This assumption results in the following equation for the flow:

$$F = \left[1 - e^{-\sinh^{-1}\left(\frac{2a}{\lambda}\right)}\right](Ap + \beta) + Ce^{-\sinh^{-1}\left(\frac{2a}{\lambda}\right)} \quad (7)$$

8

where p = the average pressure and A, B and C are defined below.

$$A = \frac{\pi\, a^4}{8\eta L} ,$$ (8)

$$B = \frac{4\pi\, a^3 RT}{3\, M_v\, L} ,$$ (9)

$$C = \frac{16\, a^3 RT}{3\, M_v\, L} .$$ (10)

All of the symbols have been defined above except for v which is:

$$\overline{v} = \left(\frac{8RT}{\pi M}\right)^{\frac{1}{2}} .$$ (11)

Equation 7 reduces to the Knudsen formula when $\lambda \gg a$ and becomes the Poiseuille equation if $a \gg \lambda$.

Equation 7 can be compared to experimental data for the flow of CO_2 through a glass capillary using the data of Knudsen [5]. The agreement between experiment and theory is quite good with the theory predicting the experimentally observed minimum at approximately the correct pressure. In figure 3, data obtained from observing the flow of N_2, O_2, and CO_2 (Lewis and Brown, unpublished results) through a gold leak into a quadrupole mass spectrometer is compared to that calculated using equation 7. The agreement between theory and experiment is excellent for the O_2/N_2 ratio and reasonable for the CO_2/N_2 ratio. (The precise radius of the pinhole
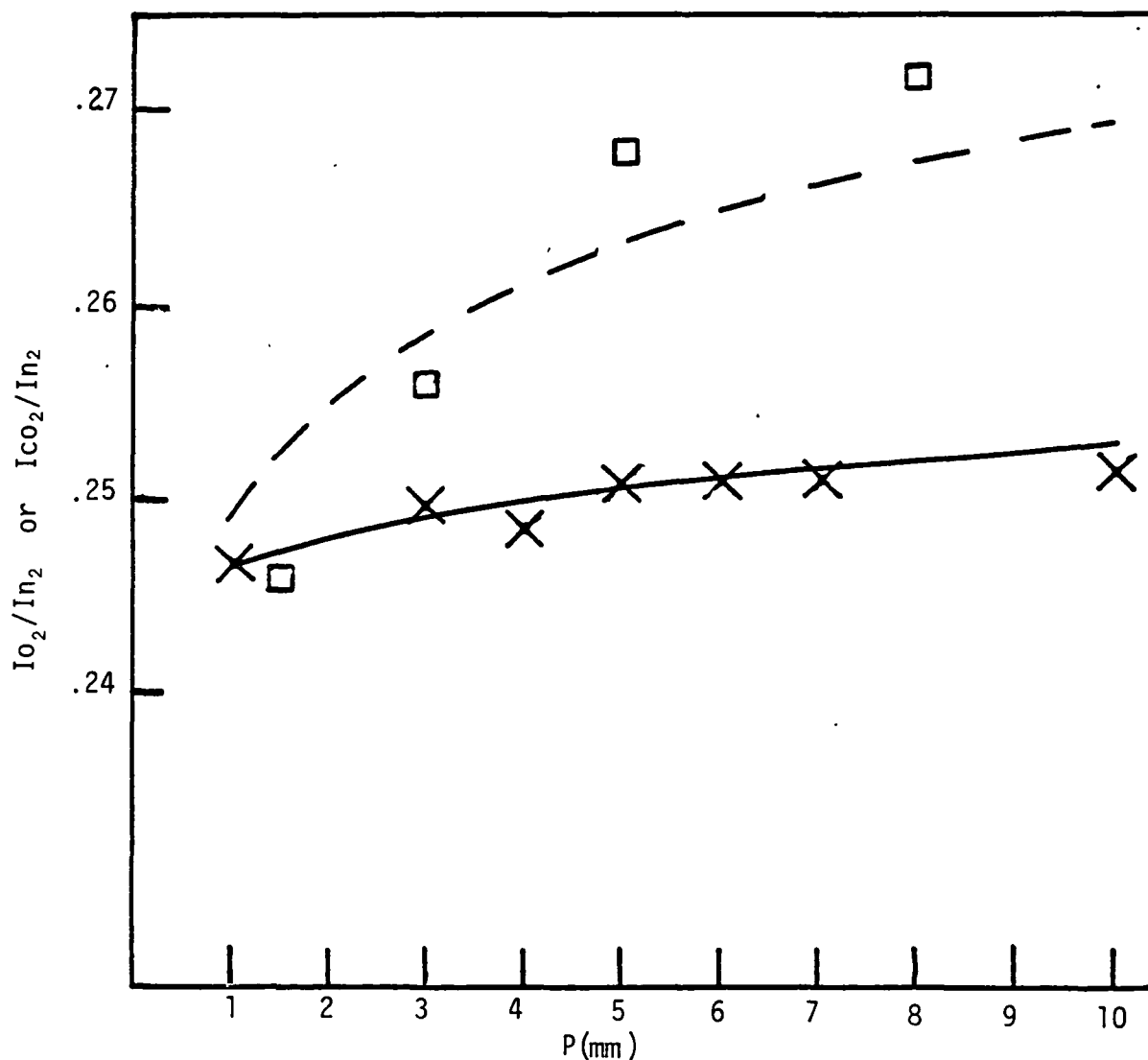
Figure 3. Comparison of the flow observed for CO_2, N_2 and O_2 in air to that calculated in equation 6. Calculated CO_2/N_2 --- calculated O_2/N_2 -, experimental CO_2/N_2O, experimental O/N x. Temperature = 300K. The calculated values assume a radius of 20µ and a length of 400µ.

and the radius of the leak were not known in this experiment.) It is apparent that, as the pressure decreases in front of the gold leak, the flow experiences a change in character as evidenced by a sharp change in slope for the ratio. This alteration in slope is due entirely to a change in nature of the flow rather than a change in composition. Any observed ratio will then have to be corrected using equation 7, or any other formalism that accounts for transition flow. As equation 7 is fairly successful in accounting for flow changes, it will be used in the remainder of this report to discuss the sampling process.

EVALUATION OF THE FLOW

The calculated flow rates for Nitrogen as a function of pressure, for different valules of L/a, are shown in figure 4. At room temperature the region of molecular flow occurs over a very small range of pressure (5 mm). At higher temperatures the range of molecular flow seems to be greater. An expansion of the data in figure 5, for a/I = .025, better illustrates the minimum in the flow at a pressure of 5 mm. At the higher temperature, 1500 K, the minimum does not occur until approximately 25 mm and is quite broad. The high temperature represents the temperatures compiled in table I for the reentry vehicle. At this temperature molecular flow is seen to occur over a wider range of temperature with the transition region extending up to 55 mm of pressure. Comparison to table I would indicate that for the lowest altitude in that table the flow would still be, at worst, transitional and not molecular.

FLOW RATES FOR MASS SPECTROMETRY

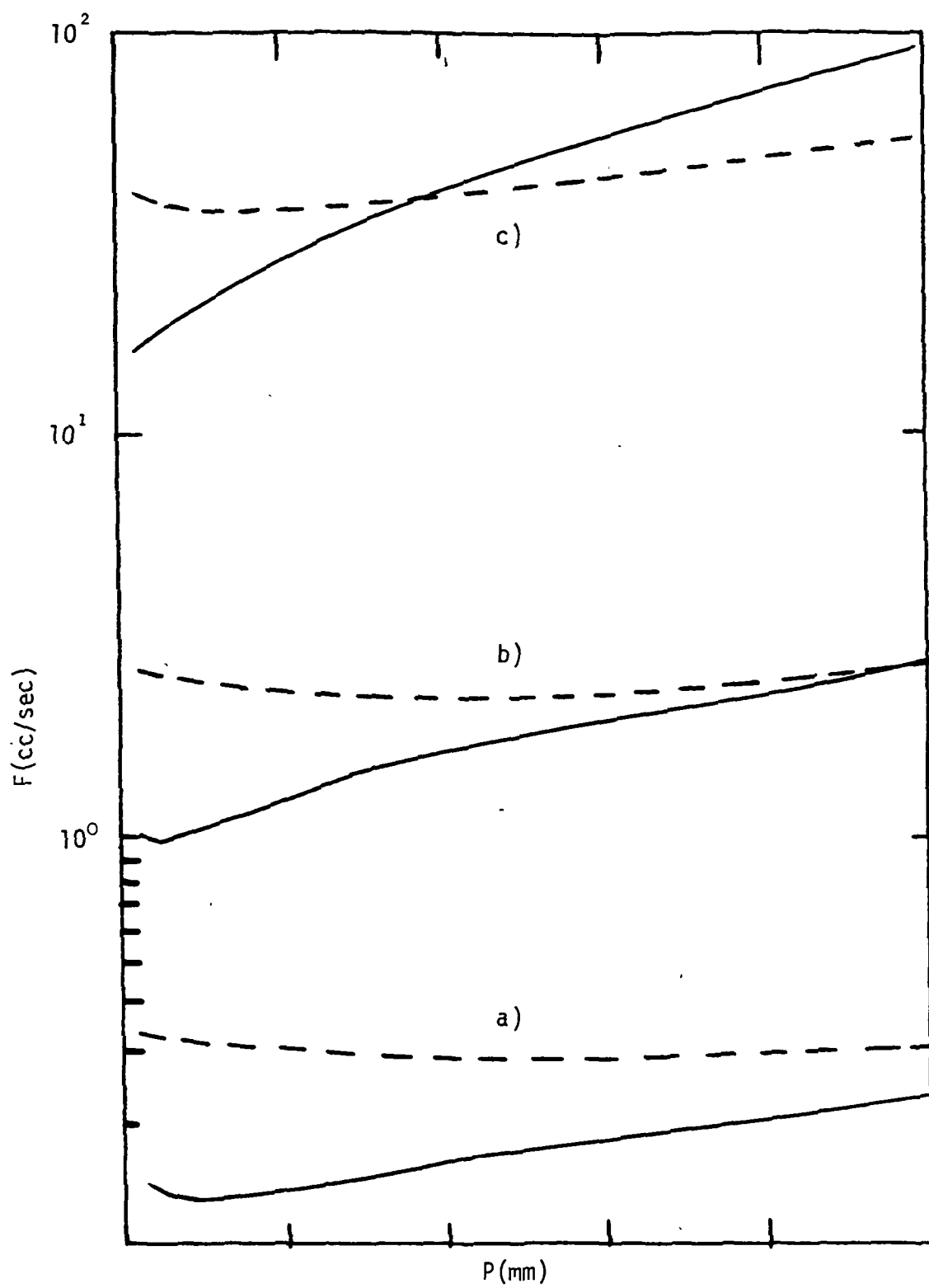The above calculations and resultant graphs are all for flow through

Figure 4. Comparison of the calculated flow rates for N_2
for equation 6. 300K (–), 1500K (---) a) L/a =
40 b) L/a = 20, c) L/a = 8. In all cases
L = 400μ.

12

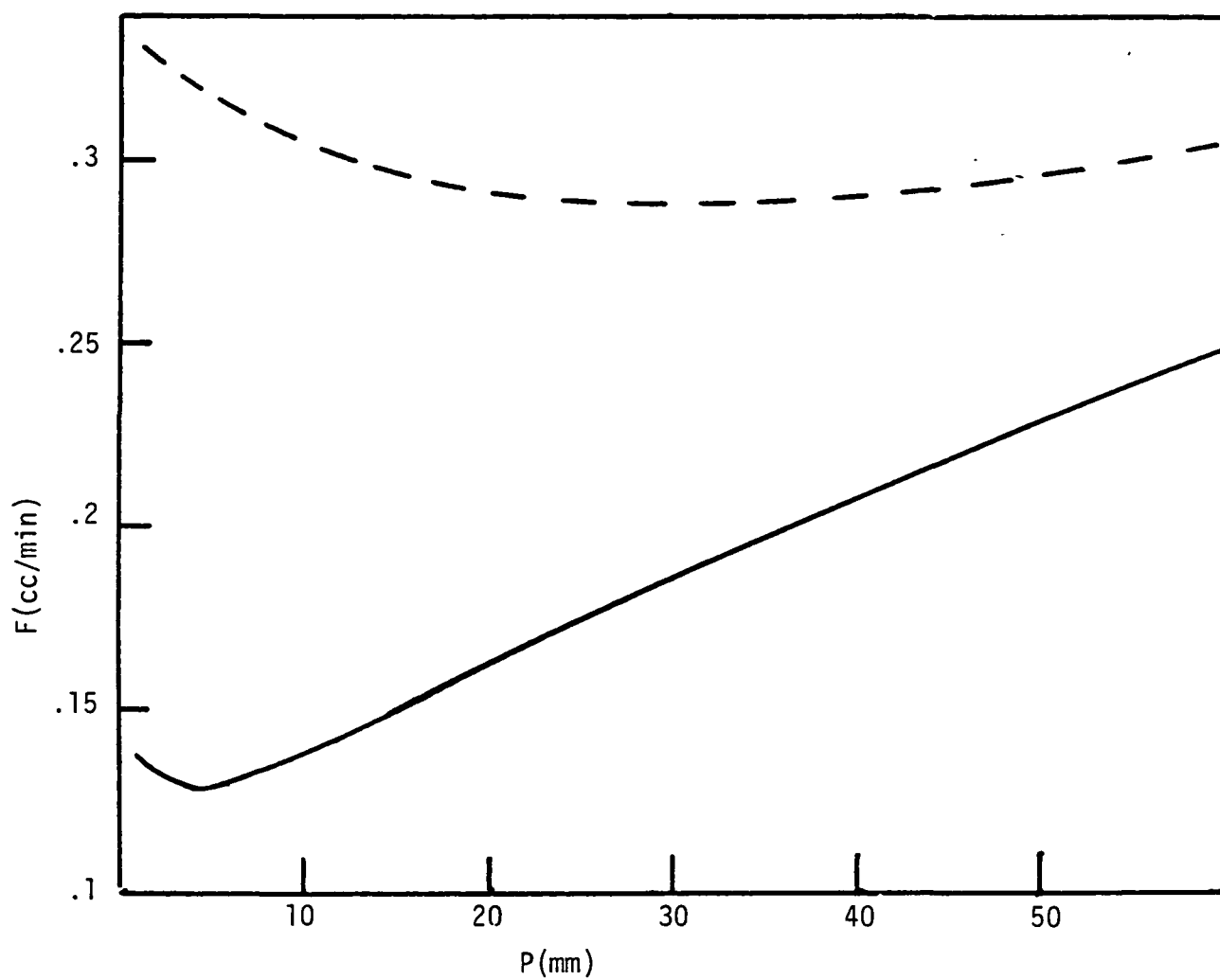Figure 5. Calculated flow rates for N_2 as a function of pressure for L/a = 40 and L = 400µ, 1500K (---) 300K (-).

13

one capillary. The proposed inlet will actually consist of an array of cap-illaries in a multi-channel plate. The number of capillary openings could vary from one thousand to well over one million. To calculate the flow through this array it is assumed, as a first approximation, that the flow through any one capillary is independent of the flow through the adjacent capillary. The total flow through the array is, then, simply the flow through one capillary multiplied by the number of capillaries. These flow rates as a function of altitude, at different L/a, are shown in figure 6. None of these flow rates is so high that it cannot be handled by conventional, readily available pumping systems, to avoid the accumulation of sample in the mass spectrometer.

EFFECT ON THE FLOW

Using the methodology developed in reference 4, the distance of sample removal from the surface was calculated. In all cases of a/L, for the conditions given in table I, the distance from the surface was no greater than 10^{-6} cm. This distance is an exceedingly small fraction of the boundary layer thickness which, at the point on the surface where the calculations were performed, is approximately 2 cm. It is quite likely that this distance lies either within, or close to the Knudsen layer. As a result removal of material through this type of effusive device should have little or no effect upon the overall stream flow.

SUMMARY

In this report the flow through a capillary opening in a surface has been analyzed. Programs have been written which will be utilized in the
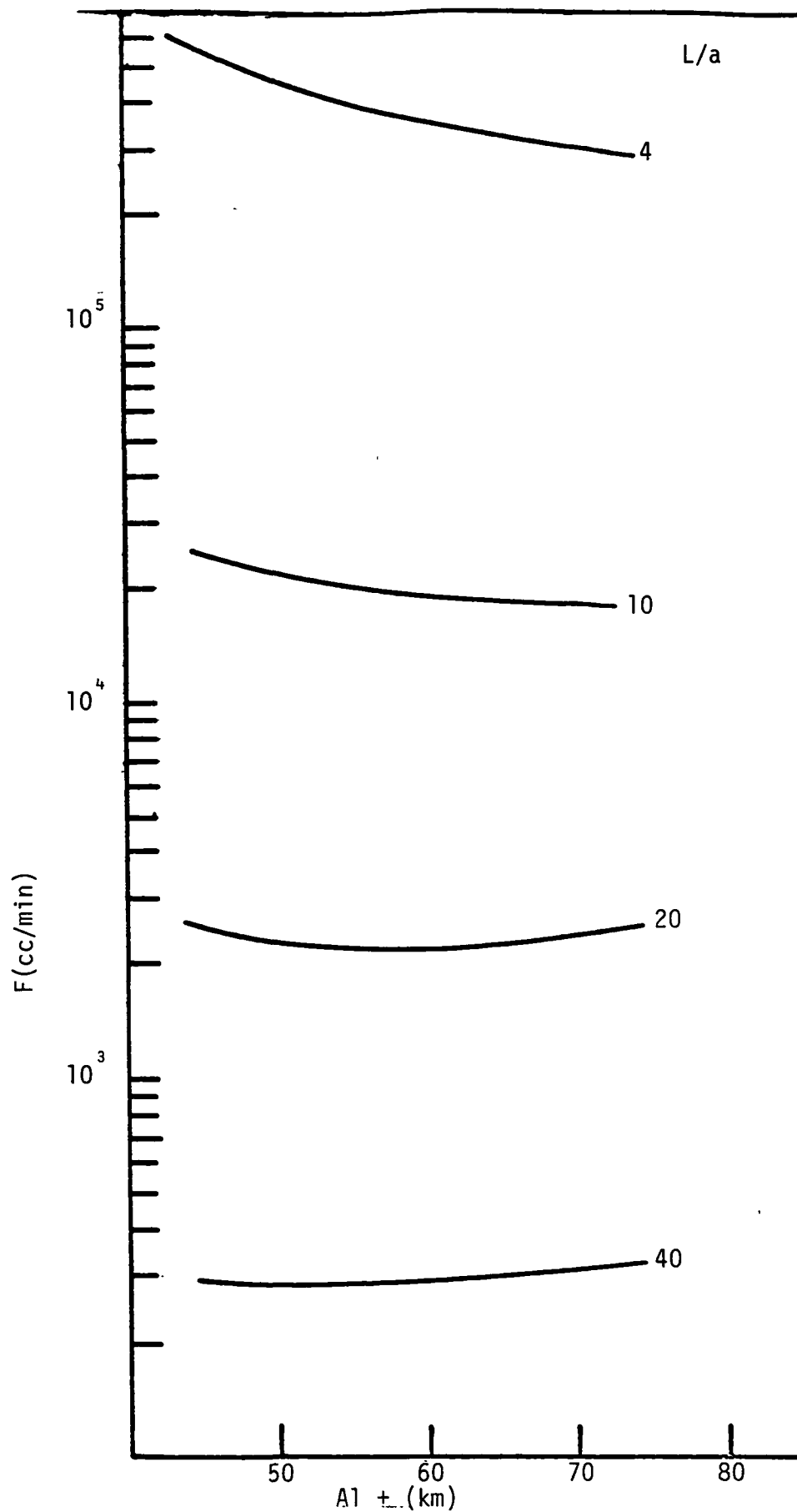
Figure 6. The calculated flow rate (in liters/min) for N_2 from equation 6 for an assembly of 1000 capillaries.

15

analysis of flow experiments which are currently proceeding in the laboratory. The major finding of this report is that for the altitudes given, and the calculated conditions, the flow through the device will, most likely be molecular or transitional. As a result most reactions caused by intermolecular collisions will occur on the exterior side of the device and not within the device itself. In addition, the material removed from the flow will be well within the boundary layer. This type of inlet would, then, be quite useful for studying surface chemistry within the boundary layer. These conclusions are amenable to laboratory testing and are currently being examined.

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