GAS FLOW THROUGH MICROGAPS

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LIST OF SYMBOLS

A = Cross sectional area

B = Parameter in Boltzmann equation (equation 3.17)

C = Constant(s), sometimes with subscripts, (Specified where used)

D = Collision integral term (equation 3.18)

E = Constant in intermolecular force expression

F = Mass flow rate

G = Constant related to effective collision cross section (equation 3.17 for example)

H = Geometrical factor (equation 2.6)

I_L = Linearized collision operator (equation 3.7)

I_{LN} = Secial linearized collision operator (equation 3.22)

J_1 = Collision integral (equation 3.14)

J_2 = Collision integral (equation 3.14)

K = Pressure gradient expression (equation 3.48)

Kn = Knudsen number λ/d

Kns = Special Knudsen number (equation 2.2)

L = Length of flow passage

M = Molecular weight

N = Number of terms in series solutions (equation 3.22 for example)

P = Pressure

P_s = Scaled pressure (equation 2.8)

P_1 and P_2 = Pressures at the ends of the flow passage

ΔP = Finite pressure difference along flow passage

LIST OF SYMBOLS (CONT.)

Q = Dimensionless flow rate $F(2kT/m)^{\frac{1}{2}}/(Ad\frac{dP}{dz})$ (equation 5.3)

$\overleftarrow{R}$ = Vector on cross section plane (Figure 1)

$\overleftarrow{\mathbb{R}}$ = Scaled vector on cross section plane (equation 4.12)

S = Point of calculation on cross section plane (Figure 1)

S_o = Point on equation trajectory line (Figure 1)

S_B = Point where equation trajectory intersects cross section boundary (Figure 1)

T = Absolute temperature

$\mathbb{T}_n$ = Special molecular velocity function (Chapter IV-C)

T_p = Dimensionless perturbed temperature (Table 1)

V_i = Molecular velocity component, V_1, V_2, V_3, V_x, V_y, V_z, etc.

$\overleftarrow{V}$ = Vector representation of molecular velocity

W_j = Function of eigenvalues q_j (equation 2.1)

$\overleftarrow{X}$ = Two dimensional vector on cross section plane (Figure 1)

$\overleftarrow{\mathbb{X}}$ = Scaled vector on cross section plane (equation 4.12)

CS = Representation of cross section plane

CSS = Representation of scaled cross section plane (equation 2.12)

CSB = Representation of boundary of CS or CSS (equation 4.1)

Per = Perimeter of cross section plane (equation 2.3)

$\mathbb{P}$ = $2\alpha u_{zp}(\overleftarrow{\mathbb{x}}) + Kd$ (equation 4.1)

a_{rl} = Factor related to perturbation eigenfunction (equation 3.12)

a_j = Single subscript representation of a_{rl} (equation 3.25)

b = Impact parameter (equation 3.1)

c = Subscript indicating colliding molecules (equations 3.1-3.4)

c_i = Peculiar (Thermal) molecular velocity component $V_i - u_i$

$\overleftarrow{c}$ = Peculiar molecular velocity vector $\overleftarrow{V} - \overleftarrow{u}$

c^2 = $c_1^2 + c_2^2 + c_3^2$

d = Characteristic dimension of flow passage, e.g., diameter of circular cross section, height of rectangular cross section, etc.

f = Velocity distribution function (equations 3.1-3.4)

f_c = Velocity distribution function of colliding molecule (equations 3.1-3.4)

f' = Velocity distribution function after collision (equations 3.1-3.4)

f'_c = Velocity distribution function of colliding molecule after collision (equations 3.1-3.4)

f_o = Local Maxwellian velocity distribution function (equation 3.27)

f_{oo} = Absolute Maxwellian velocity distribution function (equation 3.29)

g_i or g = Relative molecular velocity component $V_{ic} - V_i$

$\overleftarrow{g}$ = Relative molecular velocity vector $\overleftarrow{V}_c - \overleftarrow{V}$

h = Cross sectional height of rectangular flow passage

h_w = Nondimensionalizing term related to wall conditions $m/(2kT_w)$

i = Subscript indicating component, term in series, cell identification, etc.

j = Subscript indicating term in series, eigenvalues, etc.

k = Boltzmann's constant (or subscript where indicated)

l = Subscript for eigenfunctions and eigenvalues (equation 3.10)

m = Molecular mass

n = Number density of molecules (or subscript where indicated)

n_o = Reference number density (usually for absolute Maxwellian velocity distribution function)

n_p = Dimensionless perturbed number density (Table 1)

o = Subscript indicating local reference values

oo = Subscript indicating absolute reference values

q = Molecular separation in intermolecular force expression

q_j = Eigenvalues (equation 2.1)

r = Radius of circular cross section flow passage (or subscript where indicated)

s = Equation trajectory coordinate (equation 4.2)

t = Time

u_i = Component of mean molecular velocity $1/n\int_{V_i} V_i f dV_i$, u_x, u_y, u_z

u_p = Dimensionless perturbed mean velocity (Table 1)

u_{zp} = Dimensionless perturbed flow velocity in z direction (macroscopic velocity parallel to flow passage axis) (equation 3.44)

u_{avg} = Average cross sectional macroscopic velocity (equation 5.1)

v_i = Dimensionless molecular velocity component $V_i(m/2kT_o)^{\frac{1}{2}}$, v_x, v_y, v_z

$\vec{v}$ = Dimensionless molecular velocity vector

v^2 = $v_x^2 + v_y^2 + v_z^2$, $v_x^2 + v_y^2$, $v_1^2 + v_2^2$, etc.

w = Cross sectional width of rectangular passage (or subscript indicating wall conditions)

x_i = Physical coordinates x, y, z, or x_1, x_2, x_3, etc. (also represents dimensionless coordinates, e.g., equation 3.31)

y = Physical coordinate (refer to x_i)

z = Physical coordinate (refer to x_i), the physical coordinate in the direction of the macroscopic flow velocity

α = Size or rarefaction parameter based on model with constant collision frequency $Gn_o d(h_o)^{\frac{1}{2}}$; this is approximately related to Kn by: $\alpha \approx [(\pi)^{\frac{1}{2}}/2]1/Kn^w$

β = Angle between $\overleftarrow{X}$ and $\overleftarrow{R}$ (Figure 1)

γ = Maxwell's momentum accommodation coefficient (equations 1.1 and 2.2)

δ_{jk} = Kronecker Delta (equation 3.22)

ε = Molecular beam deflection angle in plane normal to $\overleftarrow{g}$ (equation 3.1)

ε_c = Convergence parameter (Chapter IV-D)

ζ = Slip coefficient (equation 1.1)

η = Iteration number in numerical solution for Φ (Chapter IV-D)

$\mathscr{U}$ = Polar angle for equation trajectory (Figure 1 and 2)

θ = Angle parameter for molecular beam, zero for head-on collisions (equation 3.2), or mean-free time (equations 2.11 and 2.12)

Θ = Perturbation factor related to ϕ by: $\phi = -KZ + v_z\Theta(x,y,v_i)$

Λ_n or Λ_{rl} = Eigenvalues (equation 3.9)

λ = Mean-free-path

μ = Viscosity (or a term number where indicated)

ν = Dimensionless perturbed number density for model (equation 3.34)

ρ = Mass density

σ = Molecular collision cross section

τ = Dimensionless perturbed temperature for model (equation 3.40)

Φ = Transformed variable representing u_{zp} (equation 4.12)

χ = Molecular beam deflection angle in plane containing g (equation 3.5)

ψ_{rl} = Eigenfunctions (equation 3.10)

ψ_k = Single subscript representation of ψ_{rl} (equation 3.23)

ω_i = Eigenvalues (equation 2.2)

$d\Omega$ = Solid angle into which colliding molecule is deflected (equation 3.5)

ϕ = Perturbation factor (equations 3.6 and 3.9)

ϕ_n = Eigenfunction for I_L (equation 3.9)

CHAPTER I

INTRODUCTION

Recent engineering and fabrication advances have generated the need for reliable theoretical expressions to predict moderate-pressure gas flows through very small channels. Such problems as the flow of a near-atmospheric-pressure gas through a less-than 100 microinch gap, for example, have been predictable only by empirical means. Recent works (4) (5) describe a theoretical method of handling circular and infinite-parallel-plate geometries. The present study extends and tests this theoretical method for small flow channels of rectangular and trapezoidal cross sections.

Flow problems of this type are often called "leakage phenomena". The practical concern often is not that leakage occurs, but that it can not be predicted for changed conditions. Many valves, seals, and gaskets with metal-to-metal sealing interfaces fall in this category. Even when the sealing surfaces conform well macroscopically, microscopic examination of surface finishes usually indicates the presence of small irregular-cross-section flow channels.

Small flow passages are also involved in many filtering media of the bonded crystalline material type, outgassing surfaces or pockets in vacuum systems, and vacuum seals.* In ultraminiature fluidic devices

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* Inability to optimize design of space-environment seals has been reported (15).

(14), velocity profiles, as well as flow through small rectangular passages, are of great importance.

As a flow passage is reduced in size, with other conditions constant, the continuum idealization of gas flow eventually becomes questionable. At some point in the size reduction, it becomes theoretically possible for a gas molecule to travel from one surface of the passage to another with few or no collisions. Analysis of such a situation has been of concern for over 70 years.

Although often referred to as "capillary" flow, certain aspects of this problem are more complex than usual engineering usage of the term might indicate. The practical problem is the necessity to predict flows and pressure drops for very small flow passages, but this leads directly to problems in kinetic theory and the question of how to determine the limits of applicability of continuum theory as opposed to molecular theory.

The recognized parameter for determining whether the flow should be treated as continuum or as molecular is the Knudsen number (Kn). The Knudsen number is defined as the ratio of a mean-free-path* to some characteristic dimension of the flow channel. Since this characteristic dimension is usually the channel height or diameter, it is equally valid to consider the Knudsen number a size parameter as it is to consider it (as is more commonly done) a rarefaction parameter.

With the Knudsen number very small, flow is generally considered to

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* Although inconsistencies exist in the definition of a mean-free-path for realistic molecular models, the mean-free-path concept is so useful analytically that it is almost universally retained.

be in the continuum flow regime and the classical Navier-Stokes equations are used. For the other extreme, i.e., Knudsen number very large, flow is generally considered to be in the molecular flow regime, with essentially no molecule-molecule collisions. Between these two extremes, two other flow regimes are often specified - transition flow and slip flow. In this study, these flow regimes are defined approximately by:

$10 \leq Kn$: Molecular flow regime

$1/10 \leq Kn < 10$: Transition flow regime

$1/100 \leq Kn < 1/10$: Slip flow regime

$Kn < 1/100$: Continuum flow regime

Analyses for the slip flow regime are based on the Navier-Stokes equations with slip boundary conditions. Generally these boundary conditions are meant to be first-order slip boundary conditions as given by:

$$u_z(x=0) = \zeta \left.\frac{\partial u_z}{\partial x}\right|_{x=0} \qquad (1.1)$$

where: $\zeta = C\lambda$ = Slip coefficient

$C = (\pi/4)^{\frac{1}{2}}[(2-\gamma)/\gamma]$

γ = The transfer ratio of momentum (accommodation coefficient) ≈ 1.0

Maxwell is generally credited with the concept of the slip coefficient, and Kundt and Warburg are cited for a slip-flow equation for circular tubes (10)(18). The Maxwell form of this equation is:

$$F/\Delta P = [\pi\rho/(8\mu)](1 + 4\zeta/r)r^4/L \qquad (1.2)$$

Some studies, as cited by Sreekanth (33) and Cercignani (3), have been done on the possibility of using slip boundary conditions based on

higher orders of the wall velocity gradient. Theoretically, this should extend the validity of the continuum analyses partly into the range of transition flow as defined above. Experimental evidence strongly supports the use of the first-order slip boundary conditions for the slip-flow regime as herein defined, but is less emphatic about the use of higher-order slip boundary conditions (33) (3). (It should be noted that the classical continuum analyses are based on no-slip boundary conditions because of the predictive validity of this precedure for most situations.)

For slightly higher Knudsen numbers, the flow phenomena cannot be predicted by either of the above analyses, nor can they be predicted by a molecular flow analyses. This unpredictable region, the transition-flow regime, is the major concern of this thesis.

Passages examined are of rectangular and trapezoidal cross section and are reasonable approximations of leakage channels, vacuum system passages and fluidic device channels. Transition flow through such passages has not been examined previously except by semi-empirical or empirical methods. A general governing equation is developed based on a linearized BGK model of the Boltzmann equation. This verifies that a previously derived equation (5), used for a circular cross section and proposed for an arbitrary flow cross section, is good (with some restrictions) for cross sections with sharp interior corners. A numerical procedure is developed to test the governing equation for the above flow cross sections. This procedure is less restrictive (at the cost of a minor loss in accuracy) than the procedure used by Cercignani (5) to test the applicability of the general governing equation to the circular

cross section passage. It is shown that a "correct" characteristic dimension, i.e., one which gives flow rates which match asymptotically with those in an adjacent flow regime and with empirical data for the transition regime, is not necessarily a simple across-channel dimension. Numerical predictions of flow velocities and flow rates are carried out for the above cross sections and comparisons made with semi-empirical solutions and existing empirical data.

CHAPTER II

REVIEW OF PREVIOUS WORK

Studies pertinent to gas flows through small channels tend to be concentrated on the circular cross section capillary tube and the infinite-parallel-flat-plate passage. Historically most theoretical efforts have been directed at the slip flow and molecular flow regimes. Transition flow has resisted theoretical treatment and remained the area of the experimentalist. Even relatively recent work implies that the best working equations for transition flows are empirical (22) (33).

Some of the earliest investigations were aimed at trying to explain the deviations from continuum solutions which were observed as pressures were lowered. The works of Kundt and Warburg around 1875 and Maxwell about 1879 are often conspicuously cited, e.g., (9) (10) (18). The concept of a "slip coefficient" (see equation 1.1) and the slip boundary conditions for the continuum equations originated from these works. The associated equation for slip flow through circular tubes has been given, i.e., equation 1.2. Modifications of this equation are occasionally misinterpreted as being valid for transition flow as well as slip flow (10). Part of the problem appears to be a superficial similarity of this equation to later semi-empirical equations for the transition flow regime. The situation is not clarified by the fact that Brown, et. al. (2) also correlated much capillary flow data with an empirically modified version of this same equation. Even some recent experimentation (6) seems to indicate that for some conditions this equation does

correlate the data well in spite of the fact that the flow appears to be outside the slip flow regime.

An analysis using first-order slip boundary conditions was performed by Dong for the rectangular passage (9). It is based on an earlier continuum solution which Dong credits to Cornish. This slip flow equation is:

$$F = -(4h^3w\rho/3\mu)\left\{1 + (3\zeta/h) - (6h/w)\sum_{j=1}^{\infty}\frac{\sin(q_jh)\sinh(q_jh)}{(q_jh)^4W_j[q_jh + \sin(q_jh)\cos(q_jh)]}\right\}\frac{dP}{dL} \qquad (2.1)$$

where: q_j = Eigenvalues from: $q_j\zeta = \cot(q_jh)$

$W_j = \cosh(q_jw) + \zeta q_j\sinh(q_jw)$

Ebert and Sparrow (11), apparently unaware of Dong's analysis, recently applied first-order slip boundary conditions to the Navier-Stokes equations and derived essentially the same equation for rectangular passages. Their form of this equation is:

$$F = -(8h^3w\rho/\mu)\left\{\sum_{j=1}^{\infty}h/\left[w(\omega_j)^5\right]\left[\frac{\sin^2\omega_j}{1 + 2Kns(\sin^2\omega_j)}\right]\left[(\omega_jw/h) - \frac{\tanh(\omega_jw/h)}{1 + 2Kns\omega_j\tanh(\omega_jw/h)}\right]\right\}\frac{dP}{dL} \qquad (2.2)$$

where: $Kns = C[(2-\gamma)/\gamma]\lambda/(2h)$ = Special Knudsen number (equation 6.6)

ω_j = Eigenvalues determined from: $\omega_j\tan(\omega_j) = 1/(2Kns)$