An Accurate Determination of Transitional Flow Regime Pressure Profiles in Microfluidic Crevices

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Abstract. This paper utilizes results from the higher order continuum based regularized 13-moment (R13) partial differential equations that approximate solutions from the exact Boltzmann integro-differential equation to model from first principles the gas flow in a microfluidic circular tube where the flow varies from continuum, to transitional to rarefied flow regimes along the length of the tube for various inlet/outlet pressure ratios. Results from the R13 formulation are considered as a mechanism to compare results with a Clausing equation numerical solution from rarefied gas dynamics problems that models the same flow using an integral equation formulation of the Boltzmann equation where the flow varies from a non-zero inlet upstream pressure to a zero outlet downstream vacuum pressure. We propose a mechanism to investigate the degree to which the fluid pressure/density variation along the length of a circular pipe may be utilized to develop a simplified equation set that can be applied for the numerical analysis of pressure/flow behavior in pipe networks in microfluidic problems where the Navier-Stokes equations are unsuitable.

1. Introduction

The use of pipe flow network analysis techniques as a special case of flow in ducts and pipes is commonly applied in engineering studies for the modelling of gas and water distribution. Network analysis techniques that are employed in such studies include the use of the nodal and loop methods and which in the case of steady isothermal flow are based on the simultaneous solution of the mass continuity and momentum conservation equations at discrete points within the network [10].

In general while these methods can be adopted for general use in many pipe fluid networks as special cases the assumptions on which they are based assume viscous compressible flow. In the specific case for microfluidic flow that occurs in crevices such as in certain precision pressure equipment the fluid viscous continuum assumption breaks down due to a combination of low pressures and characteristic length scales encountered. This paper will examine and develop a method to accurately determine the pressure profile within crevices when the Knudsen number is such that transitional flow regime behavior is dominant.

2. Review of Theoretical Framework for Microfluidics

The underlying macroscopic equations for fluid mechanics based on a continuum hypothesis for the conservation of mass, momentum and energy as discussed in [8] are also typically applied in microfluidics for liquids where the fluid particle size D_f is usually assumed to be $0.3\ \text{nm} \leqslant D_f \leqslant 10\ \mu\text{m}$ [3]. In rarefied gas dynamics however there is no corresponding fluid particle size limitation [13] and the gas particle size can in principle be of the magnitude of individual atoms or molecules. The underlying framework for the analysis of fluid mechanics at microscopic scales in which the continuum hypothesis does not necessarily hold true is in terms of the Boltzmann equation which is valid over all length scales.

Common approaches in solving the Boltzmann equation include moment based methods such as the regularized 13-moment equations i.e. the R13 formulation [16] which utilizes the concept of accomodation coefficients [14] and the Chapman-Enskog method [5] which is essentially based on an expansion of the distribution f as $f = f^{(0)} + \mathrm{Kn} f^{(1)} + \mathrm{Kn}^2 f^{(2)} + \cdots$ in terms of the Knudsen number $\mathrm{Kn} = \lambda/L$ where λ is the molecular mean free path and L is a characteristic length such as a pipe diameter D or channel size (width w or height h) from which commonly accepted macroscopic representations such as the Navier-Stokes equations which are a PDE first order Knudsen number approximation i.e. $\mathcal{O}(\mathrm{Kn}) = 1$ to the underlying integro-differential Boltzmann equation may be derived.

The Grad and Chapman-Enskog methods as numerical formulation approaches in solving the Boltzmann equation are valid near the hydrodynamic regime and as a result are only able to adequately address gas flows with minor rarefraction, where the rarefaction parameter δ defined as $\delta = (\sqrt{\pi}/2)/\mathrm{Kn}$ is large corresponding to the hydrodynamic limit and small corresponding to the free molecular limit. In order to consider an arbitary level of rarefaction alternative measures to cater for arbitary Knudsen numbers usually involve simplifications to the collision integral term of the Boltzmann equation and include model equations such as the Bhatnagar-Gross-Krook (BGK) simplifications. By means of either these model kinetic equations which capture the inherent behavior of the full Boltzmann equation or in terms of linearizations of the full Boltzmann equation, simulations of fluid behavior for varying levels of rarefaction are possible.

Usually for flows inbetween continuum and free molecular the slip flow regime for $0.001 \leqslant \mathrm{Kn} \leqslant 0.1$ and the transitional flow regime for $0.1 \leqslant \mathrm{Kn} \leqslant 10$ are further specified to distinguish between weakly transitional flows in which continuum PDEs such as the extended Navier-Stokes equations be adapted with higher order slip coefficients for Knudsen numbers up to $\mathrm{Kn} = 0.25$ and for which higher order Knudsen number approximations such as the Burnett equations become numerically unstable and inaccurate.

As a result there are mainly analytical/numerical results for either the continuum flow regime i.e. $\mathrm{Kn} \ll 1$ and for the free molecular flow regime i.e. $\mathrm{Kn} \gg 1$ whilst transitional flow regime results are limited. For investigations in the transitional flow regime methods are mainly restricted to either moment methods such as the R13 equations or Monte Carlo methods such as the Direct Simulation Monte Carlo (DSMC) technique [2].

In the special case of free molecular flow where the Knudsen number is large the collision integral term in the Boltzmann equation vanishes and the mass flow may be represented in terms of an integral equation commonly referred to as the Clausing integral equation in vacuum gas dynamics studies. This integral equation yields the mass flow at any cross-section for a capilliary which is typically a pipe or channel in situations where a capilliary has a vacuum pressure at the exit i.e. where the flow may be considered to be in the free molecular regime when the mean free path is larger than the capilliary diameter such that $\lambda \gg D$. Full details of the integral equation for the mass flow $J(\boldsymbol{x})$ of form $J(\boldsymbol{x}) = J_\infty(\boldsymbol{x}') + \frac{1}{\pi}\int_{\partial R(\boldsymbol{x})} J(\boldsymbol{x}') \frac{|\boldsymbol{n}\cdot(\boldsymbol{x}-\boldsymbol{x}')||\boldsymbol{n}'\cdot(\boldsymbol{x}-\boldsymbol{x}')|}{|x\boldsymbol{x}-\boldsymbol{x}'|^4} \mathrm{d}A'$ where $J_\infty(\boldsymbol{x}) = \int_{\boldsymbol{\xi}\cdot\boldsymbol{n}<0, \boldsymbol{\xi}\in\omega'} f_\infty(\boldsymbol{\xi})|\boldsymbol{\xi}\cdot\boldsymbol{n}|\mathrm{d}\boldsymbol{\xi}$ for the general case of free molecular flow with diffuse reflection in the presence of nonconvex boundaries is provided in the text of [5].

It is important to note that although this integral equation presents a means to solve for the mass flow and hence pressure distribution in capilliaries with possibly arbitary cross sectional diameters along the path of gas flow from finite pressure to vacuum pressure that it is still necessary to utilize a solution of the Boltzmann equation with suitable boundary conditions. As a result the solution of a Clausing type integral equation formulation which is exceedingly complex in the general case is usually only tractable for simple geometries such as circular pipes or rectangular channels [11].

The conventional contempory practice is to either utilize generalized slip models to the Navier-Stokes PDEs, higher order moment based formulations such the R13 equations [16], or particle based DSMC simulations for transitional flow regimes. In this paper our approach is to examine and compare results for a circular pipe with the Clausing integral equation formulation that we numerically formulate with published R13 equation results in order to study the extent to which a simplified equation set may be developed to be applied for pipe networks in which microfluidic transitional flow occurs.

3. Motivation for Study of Microfluidic Pressure Profiles

In the general case of a compressible fluid where a high pressure p_1 and low pressure p_2 are present at either ends along the length of a crevice the use of the ideal gas equation $p = \rho RT$ where $R = \mathcal{R}/M$ is the universal gas constant divided by the gas species molecular mass in the form of Boyle's law for the pressure distribution for a viscous compressible gas is form $p(z) = [p_1^2 - (p_1^2 - p_2^2)[\int_0^z h^{-3}\mathrm{d}z][\int_0^\ell h^{-3}\mathrm{d}z]^{-1}]^{1/2}$ following [6]. This solution is known to become inaccurate as $p_2 \to 0$ i.e. when the pressure is near vacuum pressures such that $p_2 \lesssim 10$ Pa. A semi-empirical equation has been reported by [15] for the flow conductance $F = ch^2 \left\{0.147f + \frac{1+2.51f}{1+3.10f}\right\}$ of a gas in a channel where c is a constant, $f = h/\lambda = hp/c_g$ is the reciprocal of the Knudsen number, λ is the mean free path of the gas as previously discussed, and c_g is a constant that depends on the gas has been used to solve for the pressure distribution in the interface gaps in precision piston-cylinder pressure balances. This approximates the solution of an isothermal one dimensional flow and has been applied to approximately model the transitional flow regime where the pressure $p(z)$ along the channel at distances z is determined from the solution of the integral equation $p = p_1 - (p_1 - p_2)\frac{\int_0^z F^{-1}\mathrm{d}z}{\int_0^L F^{-1}\mathrm{d}z}$.

This integral equation is in a form that parallels that of the Clausing integral equation approach [9] and is the motivation for investigating the feasibility of integral equation formulations of the pressure distribution in microfluidic crevices such as capillaries, where the benefit obtained is that the numerical solution of a integral equation is simpler to obtain than the solution of a differential equation.

4. Mathematical Formulation of Transitional/Molecular Pipe Flow

The underlying Clausing integral equation for the flow of a gas in a circular pipe modelled as a cylindrical tube of length L and radius a was considered by [7] in terms of the density n along the length of the tube normalized to the source density. In this model utilizing a cylindrical (R, θ, Z) coordinate system normalized coordinates $r = R/a$ and $z = Z/L$ were considered such that $0 \leqslant r \leqslant 1$ and $0 \leqslant z \leqslant 1$ and where the density $\rho(R, \theta, Z)$ along the length can be calculated as $\rho(r, z) = n(r, z)\rho_0$ from the solved for normalized density $n(r, z)$.

Under the original simplifying assumptions the density comprises of a density term $n_D(r, z)$ made of contributions from molecules which enter the tube from the source and reach the point (r, z) without colliding with the tube walls and a density term made up of contributions from molecules which have collided with the tube wall before reaching the point (r, z). As a result the total density is $n(r, z) = n_D(r, z) + n_w(r, z)$ where

$$n_D(r, z) = \frac{1}{2} - \frac{z}{2\pi}\int_0^{2\pi} \frac{\mathrm{d}\theta}{(\gamma^2\rho^2 + 4z^2)^{\frac{1}{2}}} \tag{1}$$

$$n_w(r, z) = \frac{\gamma^2}{2\pi}\int_0^{2\pi}\int_0^1 \frac{\rho^2\eta(z')\mathrm{d}\theta\mathrm{d}z'}{[\gamma^2\rho^2 + 4(z - z')^2]^{\frac{3}{2}}} \tag{2}$$

and $\rho = r\sin\theta + \sqrt{1 - r^2\cos^2\theta}$, $\gamma = \frac{2a}{L}$ and $\eta(z)$ is the Clausing function for a cylindrical channel defined in terms of the solution of the integral equation

$$\begin{aligned} \eta(z) &= \frac{1}{2\gamma}\left((\gamma^2+z^2)^{\frac{1}{2}} + \frac{z^2}{(\gamma^2+z^2)^{\frac{1}{2}}} - 2z\right) \\ &+\frac{1}{\gamma}\int_0^1 \left(1 - \frac{3|z-z'|}{2[\gamma^2+(z-z')^2]^{\frac{1}{2}}} + \frac{|z-z'|^3}{2[\gamma^2+(z-z')^2]^{\frac{3}{2}}}\right)\eta(z')\mathrm{d}z' \end{aligned} \quad (3)$$

Results are compared with the R13 based investigation in [17] who studied the effect of rarefied gas flow for varying inlet p_i and outlet pressures p_o along a circular tube and obtained expressions for the mass flow rate Q in terms of the inlet/outlet pressure ratio $P = p_i/p_o$, the gas mean free path lenth λ and a parameter α that they used to model the variation in viscosity as $\mu = \mu_0(1+\alpha\mathrm{Kn})$ as the flow changed from a continuum upstream to rarefied downstream. Their results are in the form of an implicit equation for the pressure $\bar{p} = p(x)/p_o$ in terms of the normalized distance $\bar{x} = x/L$ along the flow direction ($\bar{x} = 0$ is the inlet, $\bar{x} = 1$ is the outlet).

$$\bar{x} = 1 - \frac{\bar{p}^2 - 1 + 2\mathrm{Kn}_o[4+\bar{\alpha}(\bar{p})](\bar{p}-1) + 8[b+\bar{\alpha}(\bar{p})]\mathrm{Kn}_o^2\ln\left(\frac{\bar{p}-b\mathrm{Kn}_o}{1-b\mathrm{Kn}_o}\right)}{P^2 - 1 + 2\mathrm{Kn}_o[4+\bar{\alpha}(P)](P-1) + 8[b+\bar{\alpha}(P)]\mathrm{Kn}_o^2\ln\left(\frac{P-b\mathrm{Kn}_o}{1-b\mathrm{Kn}_o}\right)} \quad (4)$$

$$\bar{\alpha} = \frac{128}{3\pi^2(1-\frac{4}{b})}\arctan\left[4.0\left(\frac{\mathrm{Kn}_o}{\exp\{\exp[1.2271\ln(\ln(P)) - 0.6145]\}}\right)^{0.4}\right] \quad (5)$$

where $\lambda_o = \frac{16\mu_o}{5\rho_o\sqrt{2\pi RT}}$ with $R = 287$ J.kg^{-1}.K^{-1} for air and the dynamic viscosity for air is $\mu_o = 1.983\times10^{-5}$ kg.m^{-1}.s^{-1} at 300 K, $\mathrm{Kn}_o = \frac{\lambda_o}{r_0}$, and b is a second order velocity coefficient at the tube wall defined in terms of the relation $\bar{u}|_{\bar{r}=1} = -\frac{2-\sigma}{\sigma}\frac{\mathrm{Kn}}{1-b\mathrm{Kn}}\frac{\partial\bar{u}}{\partial\bar{r}}\Big|_{\bar{r}=1}$.

Further details of the values for the parameter b are sometimes ambiguous and may be obtained in the review article of [4] however it appears from the work of [12] that the b parameter is fixed by practice/definition to $b = -1$ in DSMC based simulations and further investigation is necessary to relate this DSMC slip parameter to experimental second order slip models of form $u_s = C_1\lambda\frac{\partial u}{\partial z}|_w - C_2\lambda^2\frac{\partial^2 u}{\partial z^2}|_w$. In the work of [17] the value is set as $b = -1$ for fully developed flow and $\sigma = 1$ for diffuse reflection i.e. it is assumed that the surface is smooth, that there is an absence of surface roughness and gas-surface interaction effects for simplicity, and that a linear first order slip model suffices.

In order to perform a comparison of the pressure or density distribution profiles in a circular tube of length L and radius a predicated by the R13 i.e. higher order continuum PDE formulation with that of the Clausing integral equation formulation we observe that the number density is $n = \rho/M$ where M is the particular gas species molecular mass from which a dimensionless parameter of the variation along the tube may be calculated as $\chi = p(x)/p_i$ for the PDE formulation or $\chi = n(r=0,z)/n(r=0,z=0)$ for the integral equation formulation.

5. Numerical Solution of Pressure/Density Profiles

Our approach considers [1] who provides an overview of numerical methods for the solution of nonlinear integral equations and which we then solve using the well known Nystrom method for simplicity. The essential feature is the transformation of an integral over an arbitary domain $[a,b]$ to one over $[-1,1]$ by the change of variables $t = \frac{2x-a-b}{b-a} \Leftrightarrow x = \frac{1}{2}[(b-a)t+a+b]$ so that $\int_a^b f(x)\mathrm{d}x = \int_{-1}^1 f(\frac{(b-a)t+(b+a)}{2})\frac{(b-a)}{2}\mathrm{d}t$, from which Gaussian quadrature may be applied to the integral $\int_{-1}^{1} f(x)\mathrm{d}x = \sum_{i=1}^{n} w_i f(x_i)$ where x_i are the roots of the nth-degree Legendre polynomial $P_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n$ by way of Rodrigue's formula and the weighting factor w_i are determined as $w_i = \int_{-1}^{1}\prod_{j=1,j\neq 1}^{n}\frac{x-x_j}{x_i-x_j}\mathrm{d}x$ and the Legendre polynomial explicitly calculated as $P_n(x) = 2^n\sum_{k=0}^{n} x^k\binom{n}{k}\binom{\frac{n+k-1}{2}}{n}$ and the binomial coefficient is defined as $\binom{n}{k} = \frac{n!}{k!(n-k)!}$ for $0 \leqslant k \leqslant n$. Once the quadrature formulation of the integral term is calculated in terms of a weighted summation of the function values this is substituted back into the integral equation to yield a system of simultaneous linear equations of the unknown function values which may be solved by standard techniques by which the number density as a scaled measure of the density profile may be obtained.

Based on the investigations of [7] for the Clausing integral and [17] for the regularized 13-moment differential equation formulations we restrict the numerical investigation for a pipe of radius $a = 0.75$ mm and length $L = 15$ mm i.e. for $\gamma = 0.1$ and for pressure ratios in the range $1 \leqslant P \leqslant 10 \times 10^3$ corresponding to an outlet pressure of $p_2 = 10$ Pa and an inlet pressure of $p_1 = 10\,\mathrm{kPa}$.

For simplicity a trapezoidal integration may be used in the numerical solution of the Clausing integral equation to reduce the coding effort as indicated in figure 1 over more accurate integration schemes such as Gaussian quadrature as outlined in appendix 1.

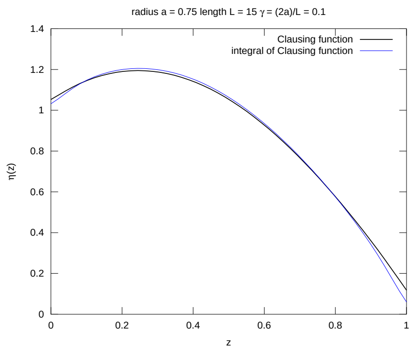

Figure 1. Clausing function solution for circular pipe geometry

6. Conclusions

A mechanism to study the transitional flow regime which occurs as an intermediate flow regime between fully continuum viscous based flow and fully particulate molecular flow through moment based differential equation solutions to the Boltzmann equation with comparison to a Clausing integral equation formulation has been proposed for the particular case of gas flow in a circular pipe.

Based on this approach the validity of integral and differential equation solutions for the pressure/density variation of flows in pipes may be studied for various geometry configurations and inlet/outlet pressure ratios with a view towards utilizing an integral equation formulation. The benefit of an integral equation such as the Clausing integral equation over differential equation solutions is that an integral equation can be more readily numerically solved without any simplifying assumptions or recourse to higher order velocity slip models for common pipe and channel geometries that occur in applied physics problems.

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Appendix A. Derivation of Numerical Scheme for Clausing Equation

Rewrite the Clausing integral for a circular tube of length L with radius a with shape parameter $\gamma = \frac{2a}{L}$ as $\eta(z) = f(z) + \int_0^1 g(z,z')\eta(z')\mathrm{d}z' \, \forall z \in [0,1]$ and apply the transformation $t = \frac{2x-(a+b)}{(b-a)}$ to the integral $\int_a^b f(x)\mathrm{d}x$ so that $\int_a^b f(x)\mathrm{d}x = \int_{-1}^1 f(\frac{(b-a)t+(a+b)}{2})\frac{b-a}{2}\mathrm{d}t$ from which with Gaussian quadrature may be approximated as $\int_{-1}^1 P(x)\mathrm{d}x = \sum_{i=1}^n w_i P(x_i)$. Substitute this approximation into the integral $\int_0^1 g(z,z')\eta(z')\mathrm{d}z'$ and observe that for $-1 \leqslant t \leqslant 1$ that $0 \leqslant \frac{t+1}{2} \leqslant 1$ so that $\int_0^1 [g(z,z')\eta(z')]\mathrm{d}z' = \int_{-1}^1 \left[g\left(z, \frac{t+1}{2}\right)\eta\left(\frac{t+1}{2}\right)\right]\frac{1}{2}\mathrm{d}t = \frac{1}{2}\sum_{j=1}^m w_j \left[g\left(z, t_j\right)\eta\left(t_j\right)\right]$ from which we have for $0 \leqslant z_i \leqslant 1$ where $i = 1, 2, \ldots, n$ for some $n \in \mathbb{N}$ that

$$\left.\begin{array}{rcl} \eta(z_1) &=& f(z_1) + \frac{1}{2}\left\{w_1[g(z_1,t_1)\eta(t_1)] + w_2[g(z_1,t_2)\eta(t_2)] + \cdots + w_m[g(z_1,t_m)\eta(t_m)]\right\} \\ &\vdots& \\ \eta(z_i) &=& f(z_i) + \frac{1}{2}\left\{w_1[g(z_i,t_1)\eta(t_1)] + w_2[g(z_i,t_2)\eta(t_2)] + \cdots + w_m[g(z_i,t_m)\eta(t_m)]\right\} \\ &\vdots& \\ \eta(z_n) &=& f(z_n) + \frac{1}{2}\left\{w_1[g(z_n,t_1)\eta(t_1)] + w_2[g(z_n,t_2)\eta(t_2)] + \cdots + w_m[g(z_n,t_m)\eta(t_m)]\right\} \end{array}\right\} \tag{A.1}$$

Setting $n = m$ we then have a matrix equation $\mathbf{A}\boldsymbol{\eta} = \mathbf{B}$ for the unknowns $\boldsymbol{\eta} = [\eta(z_1), \ldots, \eta(z_n)]^\mathsf{T}$ where the matrices are defined as $A_{ij} = \frac{1}{2}w_j g(z_i, z_j) - \delta_{ij}$ and $B_i = -f(z_i)$ for $1 \leqslant i, j \leqslant n$ and where δ_{ij} is the Kronecker function defined as $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$.