Solution of a Nonlinear Volterra Integral Equation for Concentric Annulus Channel Pressure Profiles with Mixed Viscous/Molecular Flow Regimes

Vishal Ramnath

Abstract—Pressure profiles of fluids flowing in channels and crevices are generally calculated from the conservation laws of mass, momentum and energy formulated in terms of partial differential equations which are valid in the case of continuum flows. For flows at small length scales and/or low pressures the continuum assumption breaks down and the flow physics has to utilize alternative mathematical formulations. In this paper we consider an integral equation that models the micro-fluidic gas flow in a concentric annulus channel where the flow varies from a continuum viscous flow at the inlet to a non-continuum molecular flow regime at the outlet and numerically approximate a solution to the associated system of nonlinear equations. Results of the mixed continuum/non-continuum flow pressure profile are compared to the Navier-Stokes based isothermal compressible flow pressure profile and validity accuracy limits are established for micro-fluidic simulations.

Keywords—homotopy method, micro-fluidics simulations, non-continuum gas flow, nonlinear integral equation.

I. INTRODUCTION

THE calculation of fluid pressure profiles in mechanical equipment is generally calculated in terms of solutions of the mass, momentum and energy equations which are formulated in terms of partial differential equations utilizing the assumption of a mathematical continuum [1]. For a majority of engineering applications in macroscopic problems this modeling approach is valid but in the case of small length scales and/or low pressures the assumption of a fluid continuum breaks down and alternative mathematical formulations become necessary in order to adequately capture the underlying flow physics such as gas rarefaction effects, velocity slip and temperature jumps. This deviation of real fluid flow physics from ideal continuum flows is particularly evident in micro-electromechanical systems (MEMS) such as in precision pressure equipment, micro-machining, semi-conductor manufacturing, and in certain sub-systems of existing equipment such as ink printers whose constituent components must be analyzed in terms of micro-fluidic processes and behaviors.

The defining specification for determining the degree to which a flow may be characterized as a continuum is in terms of the Knudsen number $Kn = \ell/L$ where ℓ is the mean free path length and L is a characteristic length of the system being studied where the range of the Knudsen number specifies the flow regime as approximately $0 \leq Kn \leq 0.001$ for continuum flow, $0.001 \leq Kn \leq 0.1$ for slip flow, $0.1 \leq Kn \leq 10$ for transitional flow, and $10 < Kn$ for free molecular flow following [2]. The mean free path length may be estimated from the kinetic theory of gases as $\ell = \nu\sqrt{\pi M/2RT}$ where $\nu = \mu/\rho$ is the kinematic viscosity, μ is the dynamic viscosity, ρ is the mass density, M is the molar mass, $R = 8.314472\ \mathrm{J\ mol^{-1}\ K^{-1}}$ is the universal gas constant, and T is the absolute temperature.

Alternative PDE formulations to the well known Navier-Stokes equations may be utilized for higher Knudsen numbers and include the extended Navier-Stokes equations which utilize higher order boundary and nonlinear boundary conditions, Burnett hydrodynamics, Grad equations and more recently the regularized 13-moment (R13) equations which are refinements of the original Grad equations and which are all derived from the underlying Boltzmann equation from statistical mechanics using various approaches [3]. The limitation with the use of a particular PDE choice is that the validity of the underlying equation is restricted to a range of Knudsen numbers which for example with the Burnett equations is specified as $0 \leq Kn \leq 0.3$ [4] or equivalently for a limited pressure range. As a result in the case of flows which range from a viscous continuum to a free molecular flow it is not possible to use a single governing differential equation that can adequately model the behavior of the gas. In the absence of solving the complete integro-differential Boltzmann equation, which is both mathematically complex and well as computationally expensive, alternative mathematical models to partial differential equations are possible drawing from the area of rarefied gas dynamics.

Building on earlier work reported in [5] and [6] which provides a comprehensive review of rarefied gas flows for various geometries and configurations, later research for the study of gas flows in a concentric annulus channel in the context of pressure balance pressure standards drawing on theoretical and experimental studies developed an integral

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equation for the mathematical model of the pressure profile first in the special case for parallel plate geometries in [7], and then for the more general case for spatially varying geometry profiles in [8] and [9] respectively which is the mathematical model that we will study in this paper.

II. Mathematical Model and Framework

Following [9] the model for the mixed continuum/non-continuum pressure profile in the interface gap of a piston-cylinder pressure balance as illustrated in Fig. 1 is expressed in terms of the nonlinear integral equation

$$p(x) = p_1 - (p_1 - p_2)\frac{\int_0^x [F(x)]^{-1}\mathrm{d}x}{\int_0^L [F(x)]^{-1}\mathrm{d}x} \tag{1}$$

$$F(x) = c[h(x)]^2\left[0.09837 f(x) + \frac{1+2.5117 f(x)}{1+3.1019 f(x)}\right] \tag{2}$$

$$f(x) = \frac{h(x)}{\ell(x)} = \frac{h(x)p(x)}{c_g} \tag{3}$$

In the above system of equations $p(x)$ is the unknown pressure profile that must be solved for, p_1 is the constant inlet pressure, p_2 is the constant outlet pressure, $F(x)$ is the flow conductance, $h(x)$ is the interface gap along the length of the channel through which the gas flows and is a known function, $f(x)$ is the reciprocal of the instantaneous Knudsen number Kn along the gas path in the channel, c_g is a constant for the particular choice of gas species used, and c is a constant which is not relevant as it factors out and then cancels out from the ratio of the flow conductance integrals.

The parameter c_g may be calculated by substituting and rearranging terms in the expression for the mean free path length ℓ to calculate the reciprocal of the Knudsen number as

$$f(x) = \sqrt{\frac{2M}{\pi RT}}\cdot\frac{p(x)h(x)}{\mu} \tag{4}$$

For the calculation of gas viscosity we opt to use the Sutherland formulae [1] as

$$\frac{\mu}{\mu_0} = \left(\frac{T}{T_0}\right)^{3/2}\frac{T_0 + S}{T + S} \tag{5}$$

where for dry nitrogen gas which we set as the fluid medium where $\mu_0 = 1.663 \times 10^{-5}\ \mathrm{N \cdot s/m^2}$, $S = 107$ K and $T_0 = 273$ K so that the gas viscosity calculated as $\mu = \mu_0 (T/T_0)^{3/2} \cdot (T_0 + S)/(T + S)$ at a standard temperature of 20 ºC is $\mu = 17.572918 \times 10^{-6}\ \mathrm{Pa \cdot s}$ and hence

$$c_g = \mu\sqrt{\frac{\pi RT}{2M}} = 0.006500\ \mathrm{Pa \cdot m} \tag{6}$$

which is in agreement with values reported in the literature for nitrogen gas [10] and thus demonstrates that the model may be utilized to study gas species effects for different choices of gases such as helium or argon.

For the compressible continuum gas flow as formulated

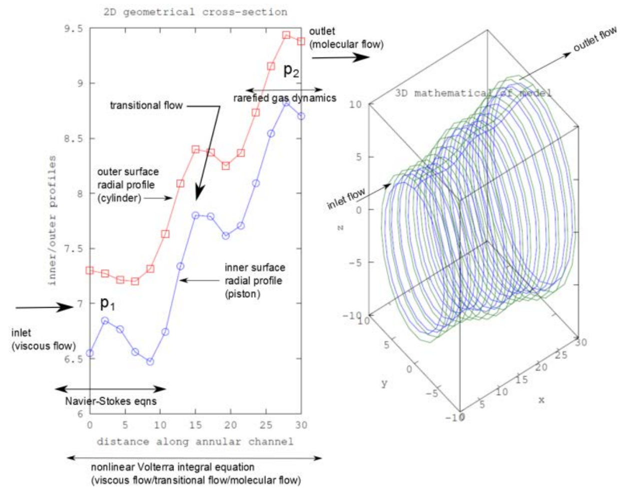

Fig. 1. Illustration of a concentric annulus channel that approximates the interface gap of a piston-cylinder pressure balance that is modeled as two concentric surfaces of revolutions from the inner and outer radial profiles

from the Navier-Stokes PDE's the pressure profile is explicitly expressed as

$$p(x) = \left[p_1^2 - (p_1^2 - p_2^2)\frac{\int_0^x [h(x)]^{-3}\mathrm{d}x}{\int_0^L [h(x)]^{-3}\mathrm{d}x}\right]^{1/2} \tag{7}$$

as discussed in [11] where the ultimate physical objective in this paper is to compare the profiles that are mathematically solved by (1) and (7) for continuum/non-continuum and continuum flows respectively.

Analyzing the form of (1) we observe that it is formulated as a nonlinear integral equation that is not directly immediately identified as either a Fredholm or Volterra integral equation since the general form for these equations of the second kind are

$$u(x) = \lambda \int_a^b K(x,y)u(y)\mathrm{d}y + f(x) \tag{8}$$

$$u(x) = \lambda \int_0^x K(x,y)u(y)\mathrm{d}y + f(x) \tag{9}$$

where $u(x)$ is the unknown function that must be determined, $K(x,y)$ is the kernel, λ is a known coefficient, and a and b are known fixed integration limits. As a result the conventional solution approaches for Fredholm and Volterra equations are not immediately accessible for (1) since it is a type of hybrid Fredholm/Volterra equation. Due to the form of (1) we immediately exclude Runge-Kutta type solutions which reformulate the integral equation as an equivalent differential equation and discount the possibility of an Adomain decomposition approach i.e. a series limit of form $u(x) = \lim_{n\to\infty}\{\sum_{i=0}^{n} u_i(x)\}$ due to the symbolic computational cost required from a computer algebra system implementation.

We observe that whilst $[F(x)]^{-1}$ is unknown since it incorporates the unknown pressure profile $p(x)$ that the integral

$$\int_0^L [F(x)]^{-1} \mathrm{d}x = C \quad (10)$$

evaluates to is a fixed but unknown constant C so that the original equation may be reformulated as

$$u(x) = \phi(x) + \lambda \int_a^x G[x, y, \phi(y)] \mathrm{d}y \quad (11)$$

where for convenience we have set $p(x) = u(x)$ as the unknown function, $f(x) = \phi(x)$ as a known source function,

$$\lambda = \frac{-(p_1 - p_2)}{\int_0^L \{F(x)\}^{-1} dx} \quad (12)$$

as an unknown constant, and

$$K[x, y, \phi(y)] = \{F(x)\}^{-1} \quad (13)$$

as the kernel for the integral equation. Equation (11) is now in the general form for a nonlinear integral equation. Considering the method of successive approximations as discussed in [12] we have

$$u_i(x) = \phi(x) + \lambda \int_a^x K[x, y, u_{i-1}(x)] \mathrm{d}y \quad (14)$$

from which it is seen that the original equation may be reformulated as a nonlinear Volterra integral equation and solved in the event that the constant λ is known.

The main challenge in applying a successive approximation is in calculating λ which may be attempted by setting $\mathrm{d}\lambda/\mathrm{d}x = 0$ by the application of Leibnitz's rule but this approach does produce any beneficial results. A practical heuristic type approach is to set $\lambda = 1$ and incorporate the $-(p_1 - p_2)/\int_0^L F^{-1} \mathrm{d}x$ integral term directly into the nonlinear kernel $K[x, y, \phi_{i-1}(x)]$ by using the compressible continuum flow pressure profile expression in (7) as a starting solution in the iteration.

Another alternative is to note that the integral equation is defined for $x \in [0, L]$ so in the presence of an unknown λ one may from an approximation functional theory perspective minimize the least squares norm of an error term $e(x)$ on $L^2[0, L]$ by defining

$$e(x) = p(x) - \left[p_1 + \lambda \int_0^L F^{-1} \mathrm{d}x\right] \quad (15)$$

and then minimizing its norm $\|e(x)\| = \left(\int_0^L |e(x)|^2 dx\right)^{1/2}$ as a simple optimization problem in terms of the parameter λ using an approximate range $\lambda \in [\lambda_{\min}, \lambda_{\max}]$ where again a starting choice of λ may be obtained from the continuum flow pressure profile in (7) and the limits for $\lambda_{\min}$ and $\lambda_{\max}$ set by convenient a prior estimates of the error between the continuum and continuum/non-continuum pressure profiles.

Although these approaches in solving the original nonlinear integral equation all have their respective merits in this paper we adopt the use of a conventional Nystrom quadrature approach, and utilize the homotopy analysis method (HAM) as a convenient potential numerical approach for controlling the convergence of the resultant simultaneous system of nonlinear equations.

For the special case in HAM problems where the homotopy analysis control parameter $\hbar$ is utilized the numerical solution of the system of nonlinear equations reduces to the use of standard solution algorithms such as Newton's method for $\hbar = 0$ or Chebyshev's method for $\hbar = -1$ as discussed in [17].

III. NUMERICAL DISCRETIZATION AND SOLUTION

The challenge of applying a conventional Gauss-Legendre numerical quadrature scheme with a weighting term $c_i = \int_{-1}^1 \prod_{j=1, j\neq i} \frac{x - x_j}{x_i - x_j} \mathrm{d}x$ so that $\int_a^b f(x) dx = \sum_{i=1}^n [\widetilde{c_i} f(\widetilde{x_i})]$ where for convenience $\widetilde{c_i} = \frac{b-a}{2} c_i$ and $\widetilde{x_i} = \frac{1}{2}[(b-a)x_i + (b+a)]$ is due to the presence of the pressure $p(x)$ in the flow conductance $F^{-1}(x)$ term which is defined in terms of the reciprocal of the Knudsen number $f(x) = h(x)p(x)/c_g$.

We observe that if one applies a Gauss-Legendre quadrature scheme then the spatial coordinate x_i when transforming the integral $\int_a^b f(x) \mathrm{d}x$ to a standard integral range $\int_{-1}^1 P(x) \mathrm{d}x$ is mapped using a simple change of variables as $t = \frac{2x-a-b}{b-a} \rightleftharpoons x = \frac{1}{2}[(b-a)t + a + b]$. The difficulty that this poses is that an evaluation of the pressure at a mapped position i.e. $p(\widetilde{x_i})$ is then necessary however the left hand side term of the unknown pressure is evaluated at an unmapped x_i whilst the right hand term in the integrals require an evaluation of the pressure at a mapped $\widetilde{x_j}$. Due to this additional complexity posed by the nonlinear Volterra type integral equation we opt for a straightforward composite trapezoidal integration algorithm with equidistant spacing for the domain as

$$x_j = a + (j-1)\delta, \delta = \frac{b-a}{n-1}, 1 \leq j \leq n, \ n \in \mathbb{N} \quad (19)$$

to avoid complicating scaling factors between unmapped and mapped coordinates as

$$\int_a^b f(x) \mathrm{d}x = \frac{\delta}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + + f(b)\right] \quad (20)$$

following the discussion in [13]. The unknown pressures p_j will be calculated for the nodes x_j where it is clear that nodes x_1 and x_n correspond to the known inlet and outlet pressures p_1 and p_2 respectively. Referring to (2), (3) and (6) we have the following system of equations as

$$u(x) = p_1 - (p_1 - p_2) \frac{\int_0^x F^{-1}(x) dx}{\int_0^L F^{-1}(x) dx} \quad (21)$$

$$F(x) = [h(x)]^2 \left[\alpha f(x) + \frac{1 + \beta f(x)}{1 + \gamma f(x)}\right] \quad (22)$$

$$f(x) = \frac{[h(x)]u(x)}{c_g} \quad (23)$$

$$[\alpha, \beta, \gamma,\ c_g] = [0.09837, 2.5117, 3.1019, 0.0065] \quad (24)$$

Applying the composite trapezoidal algorithm (20) to the above flow conductance terms we have

$$F_i = h_i^2 \left[\alpha \frac{h_i u_i}{c_g} + \left(1 + \beta \frac{h_i u_i}{c_g}\right)\left(1 + \gamma \frac{h_i u_i}{c_g}\right)^{-1} \right] \quad (25)$$

$$\int_0^L F^{-1} dx = \frac{\delta}{2}[F_1^{-1} + 2(F_2^{-1} + \cdots + F_{n-1}^{-1}) + F_n^{-1}] \quad (26)$$

$$\int_0^{x_i} F^{-1} dx = \frac{\delta}{2}[F_1^{-1} + 2(F_2^{-1} + \cdots + F_{i-1}^{-1}) + F_i^{-1}] \quad (27)$$

and substituting the above results in the following simultaneous system of nonlinear equations as

$$\varphi_1 = -u_1 + p_1 \quad (28a)$$

$$\varphi_2 = -u_2 + p_1 - (p_1 - p_2)\frac{[F_1^{-1} + F_2^{-1}]}{[F_1^{-1} + 2(F_2^{-1} + \cdots + F_{n-1}^{-1}) + F_n^{-1}]} \quad (28b)$$

$$\varphi_i = -u_i + p_1 - (p_1 - p_2)\frac{[F_1^{-1} + 2(F_2^{-1} + \cdots + F_{i-1}^{-1}) + F_i^{-1}]}{[F_1^{-1} + 2(F_2^{-1} + \cdots + F_{n-1}^{-1}) + F_n^{-1}]}, \quad 3 \le i \le n-1 \quad (28c)$$

$$\varphi_n = -u_n + p_2 \quad (28d)$$

where $\boldsymbol{\Phi}^T = [\varphi_1, \cdots, \varphi_n]^T$ and $\varphi_i = 0$ for $i = 1,2,\dots,n$ where we have used a simple trapezoidal integration $\int_a^b y(x)dx = \frac{\delta}{2}[y(a) + y(b)]$ in the special case $i = 2$. In the above system of equations the conductance terms F_i are explicitly expressed in terms of the unknown function $u(x)$ by (25).

In the above system of equations we observe the special cases for $x = 0$ that $u_1 = p_1$ and for $x = L$ that $u_n = p_2$ and as a result we only need to solve for the interior unknown pressures corresponding to indexes $i = 2,3,\dots,n-1$. As a result the system (28) will be for the solution of $(n-2)$ unknown pressures expressed in the standard form

$$\boldsymbol{\Phi}(\boldsymbol{x}) = \boldsymbol{0} \quad (29)$$

where $\boldsymbol{\Phi}(\boldsymbol{x})$ is a vector function which corresponds to the nonlinear equations in (28) and where $\boldsymbol{0}$ is zero vector.

Traditionally systems of nonlinear equations are solved by the application of Newton's method of form $\boldsymbol{x}^{(k)} = \boldsymbol{x}^{(k-1)} - \mathbf{J}^{-1}(\boldsymbol{x}^{(k-1)}) \cdot \boldsymbol{\Phi}(\boldsymbol{x}^{(k-1)})$ where $\mathbf{J}$ is the Jacobian matrix for the associated system however the main disadvantage of Newton's method apart from the high computational costs and explicit need for calculating the Jacobian matrix is that the starting solution $\boldsymbol{x}^{(0)} = [x_1^{(0)}, \dots, x_{n-1}^{(0)}]$ must be reasonably close in order to guarantee convergence.

In the present context of a single defining mathematical model that can fully capture the flow physics it is seen that the behavior of the Sutton integral equation reported in [9] actually has the gas flow deviating far from the viscous flow regime over a large portion of the concentric annular channel with the majority of the flow occurring in the molecular flow regime. As a result from this observation the starting solution pressure profile from the continuum assumption in (7) may introduce errors and a possible lack of convergence.

This potential problem is made more acute due to random fluctuations introduced in the interface gap $h(x)$ in Monte Carlo based uncertainty quantification simulations that are used to determine the associated uncertainty in the solved pressure profile in the context of pressure metrology [14] from the underlying integral equations.

Based on these considerations a less computationally intensive alternative to the traditional Newton method and optimization based modifications [15], and which importantly are more robust and more likely to guarantee convergence in the context of purely numerical based uncertainty quantification Monte Carlo simulations, are necessary.

Of various possibilities [16] that compare recent methods a recent article in [17] that utilized the homotopy analysis method for a system of nonlinear algebraic equations yielded second and third order iterative method more efficient that the normal Newton method and more importantly is well adapted for systems developed by the discretization of nonlinear integral equations. This solution approach thus potentially addresses both of the requirements in terms of solving a nonlinear integral equation and in strengthening the convergence likelihood for future uncertainty quantification simulations of the mixed flow integral equation model.

Additional details on the homotopy analysis method (HAM) is discussed in detail in [18] but the method in the context for nonlinear systems of equations $\boldsymbol{\Phi}(\boldsymbol{x}) = \boldsymbol{0}$ may be summarized as per [19] as

$$\boldsymbol{0} = \boldsymbol{\Phi}(\boldsymbol{x}^{(k)}) + \boldsymbol{\Phi}'(\boldsymbol{x}^{(k)})(\boldsymbol{y}^{(k)} - \boldsymbol{x}^{(k)})$$
$$\boldsymbol{0} = \boldsymbol{\Phi}(\boldsymbol{x}^{(k)}) + \boldsymbol{\Phi}'(\boldsymbol{x}^{(k)})(\boldsymbol{x}^{(k+1)} - \boldsymbol{x}^{(k)}) - \frac{\hbar}{2}\boldsymbol{\Phi}''(\boldsymbol{x}^{(k)})(\boldsymbol{y}^{(k)} - \boldsymbol{x}^{(k)})^2$$
$$k = 0, 1, 2, \dots \quad (30)$$

where $\hbar$ is the so-called homotopy parameter. As discussed in [17] the HAM method gives rise to Chebyshev's method for $\hbar = -1$ and in the case for $\hbar = 0$ gives rise to Newton's method. The homotopy parameter $\hbar$ is calculated using the $\hbar$-curves approach which consist of plotting the curves of possible values of $\hbar$ against the solutions of x and observing the convergence as k the order of the iteration, is increased where a flat horizontal line in the $(\hbar, x)$ curve will indicate the range of permissible values in the homotopy parameter.

In order to demonstrate the approach for the direct problem (29) we will consider the dimensional data in Table 1 below where the inlet and outlet pressures are set as $p_1 = 100$ kPa and $p_2 = 1$ kPa respectively.

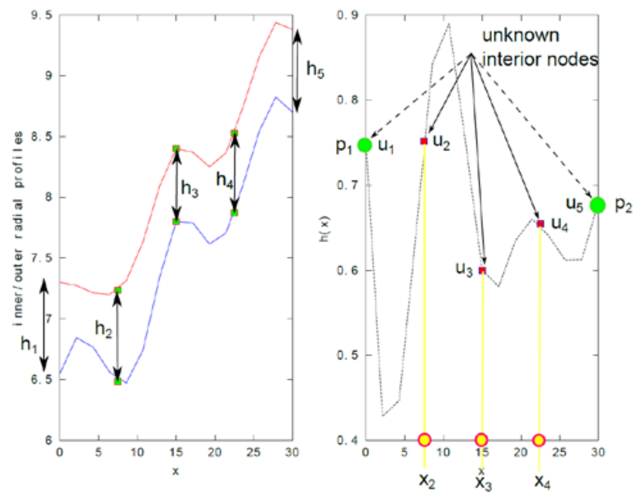

Fig. 2. Illustration of mathematical system for integral equation discretization with $n = 5$ corresponding to 5 equations with 3 unknown interior nodes and 2 boundary nodes

TABLE I
REPRESENTATIVE INTERFACIAL GAP DIMENSIONAL DATA IN A PRESSURE BALANCE

i[a]	x_i (mm)	h_i (μm)
1	0.0	0.75000
2	7.5	0.75151
3	15.0	0.60000
4	22.5	0.65408
5	30	0.68000

[a]The index i corresponding to the x vs. $h(x)$ dimensional data along the engagement length where $\boldsymbol{x} = [x_1, \dots, x_n]$ where $\boldsymbol{x} \in [0, L]$ and $h = [h_1, \dots, h_n]$

We utilize the original dimensional data plotted in Fig. 1 but due to space limitations and in order to make the analysis approach clear we will restrict the derivation of the system of equations for 5 nodes so that 3 unknown interior nodes will be solved for.

In our approach we will use the direct underlying data and not any curve fits to the expressions so the mechanism is more explicit. For the data in Table 1 there are three unknowns viz. u_2, u_3 and u_4 corresponding to spatial coordinates x_2, x_3 and x_4 since the pressures at the boundary points x_1 and x_2 are known as $u_1 = p_1$ and $u_5 = p_2$ from equation (28a) i.e. $0 = \varphi_1 = -u_1 + p_1$ and equation (28d) i.e. $0 = \varphi_5 = -u_5 + p_2$ respectively.

Expanding out in symbolic form we have three nonlinear equations in the unknowns u_2, u_3 and u_4, which read approximately as illustrated in Fig. 3 truncated to three decimal places. From the form of the system of equations it is clear that a derivative based solution techniques whilst possible is computationally expensive.

Initial calculations tabulated in table 2 indicate that the viscous continuum pressure profile calculated with (7) that uses the Navier-Stokes equations does not provide a solution for the nonlinear Volterra integral equation (1) which is able to incorporate a mixed viscous/molecular gas flow along the length of the annular channel.

$$\varphi_1 = 100000.0 - u_1$$

$$\varphi_2 = -\frac{99000.0\left(\frac{1.770\times10^{+12}}{1.137\times10^{-5}u_2+\frac{2.903\times10^{-4}u_2+1}{3.586\times10^{-4}u_2+1}}+\frac{1.777\times10^{+12}}{1.135\times10^{-5}u_1+\frac{2.898\times10^{-4}u_1+1}{3.579\times10^{-4}u_1+1}}\right)}{\frac{2.162\times10^{+12}}{1.029\times10^{-5}u_5+\frac{2.627\times10^{-4}u_5+1}{3.245\times10^{-4}u_5+1}}+2\left(\frac{2.337\times10^{+12}}{9.898\times10^{-6}u_4+\frac{2.527\times10^{-4}u_4+1}{3.121\times10^{-4}u_4+1}}+\frac{2.777\times10^{+12}}{9.080\times10^{-6}u_3+\frac{2.318\times10^{-4}u_3+1}{2.863\times10^{-4}u_3+1}}+\frac{1.770\times10^{+12}}{1.137\times10^{-5}u_2+\frac{2.903\times10^{-4}u_2+1}{3.586\times10^{-4}u_2+1}}\right)+\frac{1.777\times10^{+12}}{1.135\times10^{-5}u_1+\frac{2.898\times10^{-4}u_1+1}{3.579\times10^{-4}u_1+1}}}-u_2+100000.0$$

$$\varphi_3 = -\frac{99000.0\left(\frac{2.777\times10^{+12}}{9.080\times10^{-6}u_3+\frac{2.318\times10^{-4}u_3+1}{2.863\times10^{-4}u_3+1}}+\frac{3.541\times10^{+12}}{1.137\times10^{-5}u_2+\frac{2.903\times10^{-4}u_2+1}{3.586\times10^{-4}u_2+1}}+\frac{1.777\times10^{+12}}{1.135\times10^{-5}u_1+\frac{2.898\times10^{-4}u_1+1}{3.579\times10^{-4}u_1+1}}\right)}{\frac{2.162\times10^{+12}}{1.029\times10^{-5}u_5+\frac{2.627\times10^{-4}u_5+1}{3.245\times10^{-4}u_5+1}}+2\left(\frac{2.337\times10^{+12}}{9.898\times10^{-6}u_4+\frac{2.527\times10^{-4}u_4+1}{3.121\times10^{-4}u_4+1}}+\frac{2.777\times10^{+12}}{9.080\times10^{-6}u_3+\frac{2.318\times10^{-4}u_3+1}{2.863\times10^{-4}u_3+1}}+\frac{1.770\times10^{+12}}{1.137\times10^{-5}u_2+\frac{2.903\times10^{-4}u_2+1}{3.586\times10^{-4}u_2+1}}\right)+\frac{1.777\times10^{+12}}{1.135\times10^{-5}u_1+\frac{2.898\times10^{-4}u_1+1}{3.579\times10^{-4}u_1+1}}}-u_3+100000.0$$

$$\varphi_4 = -\frac{99000.0\left(\frac{2.337\times10^{+12}}{9.898\times10^{-6}u_4+\frac{2.527\times10^{-4}u_4+1}{3.121\times10^{-4}u_4+1}}+2\left(\frac{2.777\times10^{+12}}{9.080\times10^{-6}u_3+\frac{2.318\times10^{-4}u_3+1}{2.863\times10^{-4}u_3+1}}+\frac{1.770\times10^{+12}}{1.137\times10^{-5}u_2+\frac{2.903\times10^{-4}u_2+1}{3.586\times10^{-4}u_2+1}}\right)+\frac{1.777\times10^{+12}}{1.135\times10^{-5}u_1+\frac{2.898\times10^{-4}u_1+1}{3.579\times10^{-4}u_1+1}}\right)}{\frac{2.162\times10^{+12}}{1.029\times10^{-5}u_5+\frac{2.627\times10^{-4}u_5+1}{3.245\times10^{-4}u_5+1}}+2\left(\frac{2.337\times10^{+12}}{9.898\times10^{-6}u_4+\frac{2.527\times10^{-4}u_4+1}{3.121\times10^{-4}u_4+1}}+\frac{2.777\times10^{+12}}{9.080\times10^{-6}u_3+\frac{2.318\times10^{-4}u_3+1}{2.863\times10^{-4}u_3+1}}+\frac{1.770\times10^{+12}}{1.137\times10^{-5}u_2+\frac{2.903\times10^{-4}u_2+1}{3.586\times10^{-4}u_2+1}}\right)+\frac{1.777\times10^{+12}}{1.135\times10^{-5}u_1+\frac{2.898\times10^{-4}u_1+1}{3.579\times10^{-4}u_1+1}}}-u_4+100000.0$$

$$\varphi_5 = 1000.0 - u_5$$

Fig. 3. Illustration of the system of nonlinear equations obtained from the mixed flow nonlinear integral equation using five nodes

TABLE II
NAVIER-STOKES CONTINUUM PRESSURE PROFILE AND ILLUSTRATION OF ERRORS

i[a]	x_i (mm)	p_i (kPa)	φ_i (kPa)
1	0.0	100.00000	0.00000
2	7.5	90.70793	-5.73197
3	15.0	74.89197	-12.50938
4	22.5	50.33107	-17.07284
5	30	1.00000	0.00000

[a]The Navier-Stokes continuum pressure profile is p_i and φ_i represents the respective nonlinear equation at node i

In order to solve the mixed flow nonlinear Volterra mathematical model we must solve the associated system of simultaneous nonlinear equations in (29) which in our illustrative example is a system of five equations $\varphi_i = 0$. This problem may be converted to an equivalent optimization problem by defining a test function

$$f = \sum_{i=1}^{n} \varphi_i^2 \tag{31}$$

and then applying standard minimization routines with an approximate solution. For the illustrative example discussed the final numerical solution using a Fletcher-Reeves conjugate gradient algorithm as discussed in [21] is plotted in Fig. 4 below.

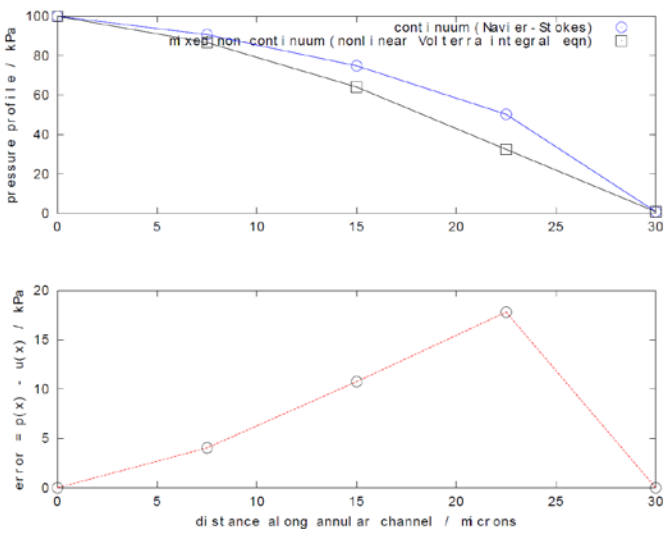

Fig. 4 Summary of the difference in pressure profiles using the viscous continuum Navier-Stokes and non-continuum mixed viscous/molecular flow integral equation

IV. DISCUSSION

In this paper we have presented the mathematical models for both viscous continuum i.e. Navier-Stokes based equations as well as mixed viscous/molecular i.e. continuum/non-continuum gas pressure flows in a concentric annular interface gap channel, and numerically solved both models for a practical industrial example. The results of the solutions indicate that one should view standard commercial CFD solutions with caution unless the underlying model has been adequately validated and verified for industrial flow simulations. Numerical strategies to solve the underlying nonlinear integral equation model have been investigated and a Nystrom quadrature approach with a homotopy analysis method modification has been identified as the most appropriate methodology for future mixed viscous / molecular continuum / non-continuum flow simulation studies as it presents the means for solving strongly nonlinear problems with the possibility for studying the convergence of the solutions.

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