Proceedings of the 4th International Conference of Fluid Flow, Heat and Mass Transfer (FFHMT'17)
Toronto, Canada – August 21 – 23, 2017
Paper No. 176
DOI: 10.11159/ffhmt17.176

A Variant of a Gradient Continuum Mechanics with Application to Flow in Microchannels

Alexander S. Liberson, Yashar Seyed Vahedein
Rochester Institute of Technology
James E. Gleason Building, 76 Lomb Memorial Drive
Rochester, NY 14623-5604, United States
asleme@rit.edu; yashar.seyed.vahedein@rit.edu

Abstract - Microscale effects become important, when the mean free path of the energy carrier becomes comparable to the characteristic length of the object. In such scale the continuum approach based on a heuristic principle of continuity is no longer valid. Modeling microflows requires to take into account the Knudsen number – the dimensionless characteristics of microscale. This is because the concept of continuity in microscale fails being applied to the finite volumes, characterized by a mean free path, or the size of a microstructural lattice. In order to account for the microstructure the higher order continuum approximation is proposed which is based on a continualization strategy inside microstructural volume and a relating variational principle. The basic generalized equations are derived and presented for fluid mechanics with applications to microstructure. Boundary conditions for the generalized mathematical model are derived based on application of a virtual work variational principle. The impact of a slip boundary condition on a velocity distribution and a mass flow rate is analyzed for a wide range of Knudsen number. It was found that the correct application of a slip boundary condition links closely to the applied gradient model. It is shown that the combination of slip boundary conditions with the classical model for the laminar flow results in a noticeable overestimation of the predicted mass flow rate. In contrast to the number of gradient models, requiring a large number of phenomenological constants, the present model requires at least one additional constant, linked to the microscale characteristic length.

***Keywords**:* microscale, gradient model, viscous flow, slip boundary conditions

1. Introduction

Different models of a non-classical mechanics and physics have been introduced using different names for the generalized continuum: Cosserat, gradient, nonlocal, nonsymmetric, microstructure, micropolar, couple stress, multipolar, micromorphic, multiscale and others. [1-6]. All these models include the higher order derivatives in mathematical formulations and additional empirical constants, whose experimental verification meets certain difficulties. The higher order gradients introduce additional degrees of freedom allowing to continualize the discrete matter, representing better as a result the discrete microstructure.

In the present paper the variant of a non-classical gradient continuum with application to the incompressible viscous flow in microscale is described. Boundary conditions for the generalized mathematical models are derived based on application of a virtual work variational principle. The impact of a slip boundary condition on a velocity distribution and a mass flow rate is analyzed for a wide range of Knudsen number. It was found that the correct application of slip boundary conditions links closely to the applied gradient model. It is shown that the combination of slip boundary conditions with the classical model for a laminar flow results in a noticeable overestimation of a predicted mass flow rate. Although the proposed model does not require the introduction of additional set of internal stresses, its basic equations are very close to the ones governing the flow of a couple stress fluid model. In contrast to our previous work [7], where theory was applied to modeling of microscale waves of a different origin in Cartesian system, in the present paper we focus exclusively on an incompressible viscous developed flow in annular ducts.

2. Microscale Averaging

Let $\partial\Omega$ be a microelement inside a volume Ω whose dimensions are significantly larger than those of $\partial\Omega$. $\mathbf{X} = (x_1, x_2, \ldots, x_N)$ is the center of mass of the underformed element, $\boldsymbol{\Xi} = (\zeta_1, \zeta_2, \ldots, \zeta_N)$ – the local coordinates in $\partial\Omega$, relative to the center of mass X. Following [7] e adopt the following procedure of averaging of the multidimensional function $\phi(\mathbf{X}+\Xi)$across the microscale volume $\partial\Omega$

$$\bar{\phi}(\mathbf{X}) = \int_{\partial\Omega} \phi(\mathbf{X}+\Xi) W(\Xi) d\Omega \tag{1}$$

where the weight function $W(\Xi)$ satisfies the normalization condition $\int_{\partial\Omega} W(\Xi) d\Omega = 1$**.** The constant value of the weight function results in the simple averaging. Presenting weight as a multidimensional Dirac delta function, $W(\Xi) = \boldsymbol{\delta}(\Xi)$, results in an equality of an averaged across microscale volume and local quantities, $\bar{\phi}(\mathbf{X}) = \phi(\mathbf{X})$**,** relating to the description of classical continuum.

Representing $\phi(\mathbf{X}+\Xi)$ as a multidimensional Taylor series arrive at (∇ is the Hamilton operator).

$$\phi(\mathbf{X}+\Xi) = \sum_{\boldsymbol{j=0}}^{\infty} \frac{\mathbf{1}}{\boldsymbol{j}!} (\boldsymbol{\Xi} \cdot \boldsymbol{\nabla})^{\boldsymbol{j}} \phi(\mathbf{X}) \tag{2}$$

equivalent to the following scalar expression

$$\phi(x_1+\zeta_1, \ldots x_N+\zeta_N) = \sum_{m_1}^{\infty} \sum_{m_2}^{\infty} \ldots \sum_{m_N}^{\infty} \frac{\partial^{m_1+\cdots m_N} \phi(x_1, \ldots x_N)}{\partial x_1^{m_1} \ldots \partial x_N^{m_N}} \prod_{j=1}^{N} \frac{1}{m_j!} \zeta_j^{m_j} \tag{3}$$

Integration according to (1) yields

$$\bar{\phi}(x_1, \ldots x_N) = \phi(x_1, \ldots x_N) + \sum_{m_1}^{\infty} \sum_{m_2}^{\infty} \ldots \sum_{m_N}^{\infty} C_{m_1 \ldots m_N} \frac{\partial^{m_1+\cdots m_N} \phi(x_1, \ldots x_N)}{\partial x_1^{m_1} \ldots \partial x_N^{m_N}} \tag{4}$$

Where

$$C_{m_1 \ldots m_N} = \int_{\partial\Omega} \prod_{j=1}^{N} \frac{1}{m_j!} \zeta_j^{m_j} W(\Xi) d\Omega \tag{5}$$

Simple averaging($W(\Xi) = 1$) boils down (5) to the following analytical expression

$$C_{m_1 \ldots m_N} = \prod_{j=1}^{N} \frac{1}{(m_j+1)!} l_j^{m_j} \tag{6}$$

in which l_j is the length scale parameter associated with the x_j direction. If all coordinates $\boldsymbol{\Xi} = (\zeta_1, \zeta_2, \ldots, \zeta_N)$ coincide with the symmetry axes inside microelement $\partial\Omega$, then odd coefficients (coefficients with odd number of indices) are equal to zero.

Consider spatial-temporal averaging of a one dimensional time dependent function $\phi(x,t)$across the microscale segment [-l, l] within the time interval [0,T].

$$\bar{\phi}(x,t) = \frac{1}{2lT}\int_0^T \int_{-l}^{l} \phi(x+\zeta, t-\tau)d\zeta d\tau \tag{7}$$

Using Taylor series expansion

$$\phi(x+\zeta, t-\tau) = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^n \zeta^k \tau^n}{k!\,n!} \frac{\partial^{k+n}\phi(x,t)}{\partial x^k t^n} \tag{8}$$

Obtain

$$\bar{\phi}(x,t) = \sum_{n=0}^{\infty}\sum_{k=0,2,4,\ldots}^{\infty} C_{kn} \frac{\partial^{k+n}\phi(x,t)}{\partial x^k t^n} \tag{9}$$

$$C_{kn} = \frac{(-1)^n l^k T^n}{(k+1)!\,(n+1)!} \tag{10}$$

The limited set of higher order derivatives is typically essential to describe the details of analyzed phenomena. Preserving the lowest two terms in the truncated series (9), arrive at equation (11).

$$\bar{\phi}(x,t) = \left(1 - \frac{T}{2}\frac{\partial}{\partial t} + \frac{l^2}{6}\frac{\partial^2}{\partial x^2}\right)\phi(x,t) + O(T^2 + L^4) \tag{11}$$

which is asymptotically equivalent to

$$\phi(x,t) = \left(1 + \frac{T}{2}\frac{\partial}{\partial t} - \frac{l^2}{6}\frac{\partial^2}{\partial x^2}\right)\bar{\phi}(x,t) + O(T^2 + L^4) \tag{12}$$

It will be shown that the continualization procedure (12), being applied to different physical phenomena, results in generalized gradient models, which are unconditionally stable, and preserve Galilean invariance.

3. Incompressible Fluid Flow in Microscale

The classical Newtonian incompressible fluid model is governed by the following system of Navier-Stokes equations ($\frac{D}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{U}\cdot\boldsymbol{\nabla}$ - is a substantial derivative).

$$\frac{D\boldsymbol{U}}{Dt} + \frac{1}{\rho}\boldsymbol{\nabla} p = \boldsymbol{\nu}\Delta\boldsymbol{U}$$
$$\nabla\cdot\boldsymbol{U} = 0 \tag{13}$$

subject to the no slip wall boundary conditions. We assume that microstructure affects predominantly spatial distribution of velocity vector, and does not affect pressure. Applying multidimensional generalization of the continualization procedure (12) by substituting $\boldsymbol{U}$ for $\boldsymbol{U} - \frac{l^2}{6}\Delta\boldsymbol{U}$ into the momentum balance equation, obtain

$$\frac{\mathrm{D}(\boldsymbol{U} - \frac{l^2}{6}\Delta\boldsymbol{U})}{Dt} + \frac{1}{\rho}\boldsymbol{\nabla} p = \nu(\Delta\boldsymbol{U} - \frac{l^2}{6}\Delta\Delta\boldsymbol{U}) \tag{14}$$

$$\nabla\cdot\boldsymbol{U} = 0 \tag{15}$$

For unidirectional flow between two parallel plates (plane Poiseuille flow), the velocity field $\boldsymbol{U} = (u(x,y), 0, 0)$ automatically satisfies the continuity equation (15). The momentum balance (14) reduces to the following Helmholtz equation (μ is a dynamic viscosity, prime – derivative by axial coordinate, $l_0 = l/\sqrt{6}$)

$$l_0^2 \Delta \mathrm{V} - \mathrm{V} + \frac{1}{\mu} P' = 0, \qquad V = \Delta u \tag{16}$$

To specify correctly boundary conditions we apply the virtual work variational principle (Γ – boundary of a cross section domain Ω, n – normal to the boundary contour)

$$\begin{gathered} \oiint \left(l_0^2 \Delta \mathrm{V} - \mathrm{V} + \tfrac{1}{\mu} P' \right) \delta u d\Omega = \\ \oiint \left(l_0^2 \mathrm{V} \delta \Delta u + \nabla u \cdot \delta \nabla u + \frac{p_x \delta u}{\mu} \right) d\Omega + \int_\Gamma \ [(l_0^2 \tfrac{\partial V}{\partial n} - \tfrac{\partial u}{\partial n}) \delta u - l_0^2 V \delta \tfrac{\partial u}{\partial n}] \mathrm{d}\,\Gamma \end{gathered} \tag{17}$$

It follows from (17) that for the free surface boundary conditions should comply with the following

$$\frac{\partial u}{\partial n} = \frac{\partial V}{\partial n} = 0 \tag{18}$$

The kinematic condition on a wall, applied to the velocity component u should be combined with the natural boundary condition, relating to the Laplace equation

$$\mathrm{V} = \Delta \mathrm{u} = 0 \tag{19}$$

We introduce the slip boundary conditions, which accounts for the first two terms in a truncated Taylor series expansion (3)

$$\mathrm{u}(R) + l u_r(R) = 0; \tag{20}$$

Symmetry conditions for the annual duct are utilized at r=0 (axis of symmetry), setting all odd derivatives to zero

$$u_r(\mathrm{r{=}0}) = V_r(\mathrm{r{=}0}) = 0 \tag{21}$$

For the polar system of coordinates $\Delta \mathrm{u} = \frac{1}{r}(r u')'$. Integrating system (16)-(21), the scaled velocity component $\bar{u} = -\frac{\mu u}{R_0^2 P'}$ can be presented as the following

$$\bar{u} = \frac{1}{4}\left[\left(\frac{r}{l_0}\right)^2 - 1\right] + l_0^2 \left(\frac{I_0(\left(\frac{r}{l_0}\right)}{I_0(\left(\frac{1}{l_0}\right)} - 1 \right) + l \left(\frac{1}{2} - l_0 \frac{I_1(\left(\frac{1}{l_0}\right)}{I_0(\left(\frac{1}{l_0}\right)} \right) \tag{22}$$

in which I_0 and I_1 are the modified Bessel functions [9]

The case $l_0 = l = 0$ corresponds to the classical circular Poiseuille flow [8]. Setting $l = 0$ we arrive at the solution for the gradient model with no-slip boundary conditions [6]. The volume flow rate can be obtained by integrating (35) across the normalized distance [0,1].

Fig. 1 presents velocity as a function of a normalized coordinate r versus Knudsen numbers, which is the ratio of a microscale length to the radius, Kn=l. Results presented on a left are based on the described gradient model accounting for the slip boundary conditions (equation (36)). Distributions on a right correspond to the classical laminar model coupled with the slip boundary conditions (equation (36), the first and the third terms only). Velocity distributions predicted by both models are monotone functions of a Kn number, although it is more affected by Kn number in the simplified model (the chart on a right). The line Kn=0 relates to the classical Poiseuille solution with no-slip boundary conditions. Figure 2 displays variation of a flow rate as a function of a Knudsen number based on a gradient model subject to the slip boundary conditions (circle dots), and a classical laminar model, coupled with the slip boundary conditions (square dots). The mass flow rate is a monotone function of a Knudsen number in both cases, although the simplified classical model noticeably overestimates the flow rate. The case $Kn = 0$, corresponds to the classical Poiseuille solution satisfying the no-slip boundary conditions.

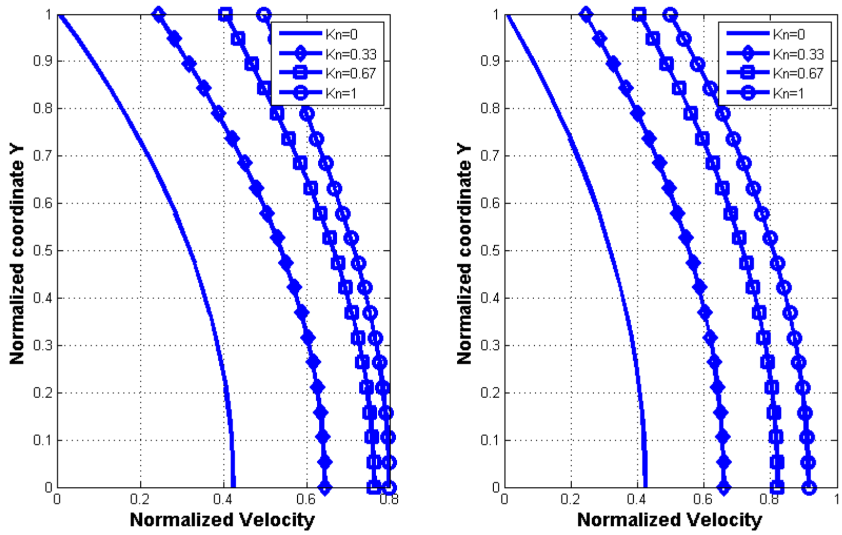

Fig. 1: Velocity profile based on a gradient model (left) and a classical model (right).

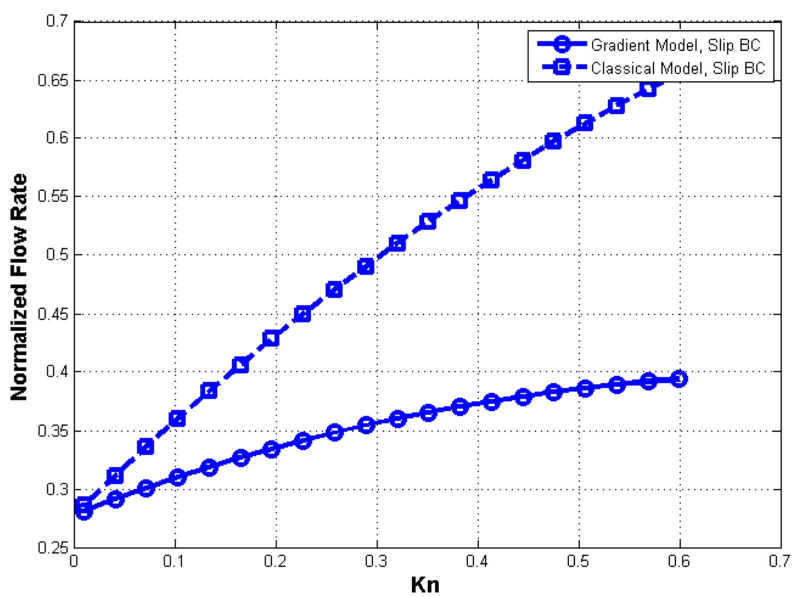

Fig. 2: Mass flow rate versus Knudsen number.

4. Conclusion

A new version of a non-classical gradient continuum is presented, which results in a higher order differential model with application to microscale fluid mechanics. Boundary conditions for the generalized mathematical model are derived based on application of a virtual work variational principle. The impact of a slip boundary condition on a velocity distribution and a mass flow rate is analyzed for the wide range of Knudsen number. It was found that the correct application of a slip boundary condition links closely to the applied gradient model. It is shown that the combination of slip boundary conditions with the classical model of a laminar flow results in the noticeable overestimation of a predicted mass flow rate.

References

[1] H. Askes, A. S. J. Suiker, L. J. Sluys, "A classification of higher order strain-gradient models-linear analysis," Archive of Applied Mechanics, vol. 72, no. 2-3, pp. 171-188, 2002.

[2] A. S. Eringen, "Micro Continuum Field Theory," Springer Verlag, New York, 1999.

[3] A. S. Eringen, "Micropolar Theory of Liquid Crystals," in *J. F. Johnson and R. S. Porter, Eds., Liquid Crystals and Ordered Fluids,* vol. 3, Plenum Publishing, New York, 1978

[4] G. Lukaszewicz, "Micropolar Fluid Theory and Applica-tions," Birkhauser, Boston, 1999.

[5] P. Power, "Bio-Fluid Mechanics, Advances in Fluid Mechanics," W.I.T. Press, UK, 1995.

[6] V. K. Stokes, "Theories of Fluids with Microstructure," Springer-Verlag, Berlin, 1984.

[7] A. Liberson. "Microscale: Wave Propagations Modeling Using a High Order Gradient Continuum Theory," *Encyclopedia of nanomechanics*, in press, 2017.

[8] H. Schlichting, *Boundary Layer Theory*. John Wiley & Sons, 2011.

[9] M. Abramowitz and I. Stegun (Editors), *Handbook of Mathematical Functions, with Formulas, Graphs, and Mathematical Tables*, [Online]. Available: http://people.math.sfu.ca/~cbm/aands/abramowitz_and_stegun.pdf