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A boundary integral equation formulation for the thermal creep gas flow at finite Peclet numbers

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ABSTRACT

The integral equation formulation developed previously by the authors to study isothermal micro flows under shear slip boundary condition is extended in this work to consider the case of non-isothermal micro gas flows with thermal creep effects at finite Peclet numbers. The effect of thermal creep over the flow patterns with and without considering the effect of shear slip is investigated in detail using a boundary element method. In this work the boundary integral approaches for both fluid velocity and temperatures fields are used to solve the problem of shear-driven cavity flow at finite Peclet number. This is obtained by considering the diffusive-convective heat equation using the Dual Reciprocity Method to transform the corresponding volume integral of the convective terms into equivalent surface integrals.

1. Introduction

Micro Electro Mechanical Systems (MEMS) based on the thermal creep phenomenon, like Knudsen-type compressor and gas vacuum pumps, can operate subject to temperature gradients without moving parts [1]. Gas flows at micro scale conditions are characterized by the Knudsen number [2], which is defined as the ratio between the mean free path of the molecules, λ, and the characteristic length scale of the flow, h, (the fluid gap in our case)

$$Kn = \frac{\lambda}{h} \tag{1}$$

The Knudsen number provides a measure of how rarefied is the gas flow and according to its magnitude four different formulations of the governing equations and boundary conditions can be defined [3]: The classical continuum representation holds when $Kn < 10^{-3}$ described by the Navier–Stokes system of equations and the no-slip boundary conditions. As the fluid gap decreases, the fluid moves into the slip regime; in the regime $10^{-3} < Kn < 10^{-1}$, the Navier–Stokes system of equations for the flow motion remains valid in a continuum description, but a first order slip boundary condition on the fluid solid interface becomes relevant. At $10^{-1} < Kn < 10^{1}$ a transition regime appears, where a molecular behaviour is present and higher order corrections and model variations are needed to estimate the flow behaviour. As Kn varies, the Navier–Stokes system of equations requires the implementation of second-order slip boundary conditions to adequately predict the flow behaviour; this approximation is valid only for $Kn < 1$. At higher Kn, the Navier–Stokes system of equations should be replaced by other conservation equations, like quasi-hydrodynamic (QHD) equations, quasi-gas-dynamic (QGD) equations or higher-order fluid dynamics models like the Burnett equations [4]. The molecular approach is required for $Kn > 10$. However, most of the micro gas flow applications reported in the literature operate in the slip flow regime, satisfying the continuum hypothesis (Navier–Stokes system of equations) with the corresponding first-order slip boundary conditions [4].

In the simulation of micro-fluid gas flows, besides considering the shear slip, with the tangential fluid velocity at the solid boundaries proportional to the tangential projection of the wall shear rate, the effect of thermal creep also needs to be considered, where due to tangential temperatures gradients along the contour boundaries of the gas are forced to slip over the solid surfaces from colder to hotter regions [5]. The Maxwell boundary condition [6] accounts for the slip velocity due to tangential shear rate and tangential heat flux effects.

Maxwell boundary condition relates the tangential gas velocity, u_s^f, at the boundary contours, i.e., the fluid velocity tangential to the wall, to the tangential shear stress and the tangential heat flux. In terms of a characteristic velocity U, the length scale h and a characteristic pressure $\mu U/h$, the slip condition can be written in

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dimensionless form as

$$u_s^f - U_s^w = L_s \dot{\gamma}_s + L_{sT}(-q_s) \tag{2}$$

where U_s^w is the wall velocity, $q_s = (-\partial T/\partial x_i)s_i$ is the dimensionless tangential heat flux at the boundary contours, and

$$\dot{\gamma}_s = \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) n_j s_i = \left(\frac{\partial u_i}{\partial n} s_i + \frac{\partial u_j}{\partial s} n_j\right) \tag{3}$$

is the tangential shear rate, where n_i and s_i are, respectively, the i components of the normal and tangential vectors to a boundary surface.

In expression (2), the coefficient L_s corresponds to the shear slip [7] and the coefficient L_{sT} to the thermal creep [4]. The proportionality constant is called slip length, L_s (dimensionless slip length in this case), and represents the hypothetical outward distance at the wall needed to satisfy the no-slip flow condition. Additionally, L_{sT} is a dimensionless constant that relates the thermal creep effect with thermo physical properties defined at the fluid–solid interface, like the intermolecular collision condition, the compressibility and the specific heat of the gas [4].

In the slip flow region, the energy equation is also subject to a temperature jump condition at the boundary contours to account for the thermal creep effect, [4], described by the following boundary condition:

$$T^f - T^w = L_T(-q_n), \tag{4}$$

with T^f as the fluid temperature, T^w as the wall temperature, and $q_n = (\partial T/\partial x_i)\, n_i$ as the dimensionless normal heat flux to the surface and L_T is a constant coefficient. This boundary condition was used by Lockerby and Reese [8] to provide a good agreement in wall shear stress and heat flux with Direct Simulation Monte Carlo (DSMC) results up to $Kn = 0.1$. When $Kn > 0.1$ only qualitative agreement can be reached and higher order boundary conditions have to be used [9]. However, in the range of $10^{-3} < Kn < 10^{-1}$ the boundary condition (2) in combination with temperature jump condition (4) can be used to analyse several micro gas flow applications [4].

In this work, an integral equation formulation based on the normal and tangential projections of the direct boundary integral representation formula for the Stokes velocity is employed to numerically simulate the non-isothermal micro gas flows subject to shear slip and thermal creep effects. A difficulty encountered when extending this type of approach to non-isothermal conditions with thermal creep effect arises when evaluating the tangential derivative of the temperature integral representational formula at the solid–fluid interface, resulting in a Cauchy singular integral that needs to be evaluated in the sense of its principal value. In this work, this singularity is removed by subtracting from the original temperature integral equation the integral representation formulae of a known potential field, having at a given collocation point the same field value and gradient of the original temperature field. The resulting boundary integral formulation is used to solve the problem of the shear-driven cavity flows at finite Peclet number by considering the diffusive-convective heat equation using the Dual Reciprocity Boundary Element Method (DR-BEM) to transform the corresponding volume integral of the convective terms into equivalent surface integrals. The mentioned subtraction of singularities approach is used to determine the tangential derivative of the corresponding wall temperature.

2. Integral formulation for slip flow with thermal creep at finite Peclet numbers

The Stokes velocity field at a point x in a closed domain Ω (with boundary Γ) filled with a Newtonian fluid can be defined in terms of the following Green's integral representation formula [10]:

$$c(x)u_i(x) - \int_\Gamma K_{ij}(x,y)u_j(y)d\Gamma + \int_\Gamma u_i^j(x,y)f_j(y)d\Gamma = 0, \tag{5}$$

where c is a coefficient function depending only on the geometry of Γ, and K_{ij} and u_i^j are the fundamental solutions of the Stokes system. The normal and tangential projections of the above boundary integral formula can be obtained after multiplying Eq. (5) by the local normal and tangential vectors n_i and s_i, at a surface point, and expressing the velocity and surface traction vectors in terms of their corresponding normal and tangential components, $(u_n,\ u_s)$ and $(f_n,\ f_s)$, i.e., $u_i(x) = u_n(x)n_i + u_s(x)s_i$ and $f_i(x) = f_n(x)n_i + f_s(x)s_i$, with $u_n = u_j n_j$, $u_s = u_j s_j$, $f_n = f_j n_j$ and $f_s = f_j s_j$.

Using the boundary condition (2) into the corresponding normal and tangential projections of the direct boundary integral representation formula, the following surface integral equations are obtained:

$$\begin{aligned}
&\int_\Gamma u_i^j(x,y)(f_n(y)n_j(y) + f_s(y)s_j(y))n_i(x)d\Gamma - \int_\Gamma K_{ij}(x,y)L_S\, f_s(y)s_j(y)n_i(x)d\Gamma \\
&\quad = -c(x)U_n^w + \int_\Gamma K_{ij}(x,y)(U_j^w(y)\ n_i(x))d\Gamma \\
&\qquad + \int_\Gamma K_{ij}(x,y)\left(L_{sT}\frac{\partial T(y)}{\partial s_j(y)}s_j(y)n_i(x)\right)d\Gamma
\end{aligned} \tag{6}$$

and

$$\begin{aligned}
&c_i(x)L_S\, f_t(x) + \int_\Gamma u_i^j(x,y)(f_n(y)n_j(y) + f_s(y)s_j(y))s_i(x)d\Gamma \\
&\quad - \int_\Gamma K_{ij}(x,y)L_S\ f_s(y)\ s_j(y)\ s_i(x)d\Gamma \\
&\quad = -c_i(x)U_s^w + \int_\Gamma K_{ij}(x,y)(U_j^w(y)\ s_i(x))d\Gamma \\
&\qquad + \int_\Gamma K_{ij}(x,y)\left(L_{sT}\frac{\partial T(y)}{\partial s_j(y)}s_j(y)s_i(x)\right)d\Gamma,
\end{aligned} \tag{7}$$

where $U_j^w = U_n^w n_j + U_s^w s_j$ and the last term on the right-hand side of both equations accounts for the thermal creep due to the tangential temperature gradient at the wall boundaries. As can be observed, in our formulation we are neglecting natural convection effects due to the boundary temperature differences to focus our attention only to the effect of thermal creep.

The limiting value of the integral kernels in (6) and (7), as the radius r tends to zero, presents only logarithmic singularities coming from the kernels $u_i^j(x,y)n_j(y)n_i(x)$ and $u_i^j(x,y)s_j(y)s_i(x)$; for more details see [11]. These two equations form a system of surface integral equations for the unknowns $(f_n,\ f_s)$. The corresponding values of $(f_1\ ,\ f_2)$ are directly obtained from the relation $f_i(x) = f_n(x)n_i(x) + f_s(x)s_i(x)$. The solution of Eqs. (6) and (7) under the thermal creep condition requires the evaluation of the temperature field, with the aim of obtaining the tangential temperature gradient, $q_s = \partial T/\partial s$, to account for the thermal creep effect at the boundary contours.

3. Integral formulation for the normal heat flux

The temperature field is found by solving the steady state energy equation

$$\mathrm{Pe}\ (\vec{u}\ .\nabla \mathrm{T}) = \nabla^2 T \tag{8}$$

where $Pe = hU/D$ is the Peclet number, and D the thermal diffusivity coefficient.

Eq. (8) can be seen as a Poisson equation with a non-homogenous term given by the convective component of the above energy equation, whose integral representation formulae can be found by applying Green's second theorem, leading to the