Ellipsoidal statistical Fokker-Planck simulation of thermally induced gas flow in a ratchet microchannel

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Abstract. We present numerical simulation results of thermally induced gas flow in the gap between a ratchet surface and a moving wall using the recently proposed ellipsoidal statistical Fokker-Planck (ESFP) algorithm. In this algorithm, the evolution of individual molecular velocity is modelled as a continuous stochastic process, and the corresponding Langevin equation is implemented in a particle Monte Carlo manner. The simulation aims at the calculation of the thermally induced shear stress acting on the top wall. In the transition regime, the mechanical power output and thermodynamic efficiency are calculated for various moving speeds of the upper wall and inclination angles of the specular surface. The proposed method facilitates the evaluation of the efficiency of converting transverse heat flux across the channel into the tangential propelling force for this device. The dependence of efficiency of the inclination angle is identified, and the optimal efficiency is found to be not much different from that in the free molecular regime.

1. Introduction
Transport phenomena occurring in the scales comparable to the mean free path of gas molecules can be well described by the kinetic theory of gases, where the Boltzmann equation provides an accurate description of the evolution of velocity distribution of gas molecules. In this rarefied regime, various types of thermally induced flow are observed based on numerical simulations and experimental investigations [1–4] since a long time ago. The scenarios include thermal creep flow, thermal edge flow and thermal stress slip flow, depending on the specific temperature and boundary conditions. Thermal creep flow velocity along a channel with varying temperature is proportional to the tangential temperature gradient [1], which limits the application of such flows.

Recently it has been shown that thermal creep flow can also be produced in a periodically structured channel in the absence of surface temperature gradient. This induced flow in the horizontal direction and the resultant shear force on the confining boundary is ascribed to the participation of a specularly reflecting surface as shown in Fig.1 (a). Almost coincidentally, thermal creep mechanism was claimed as the origin of the self-propelling Leidenfrost droplets [5, 6], where the ratchet channel is nevertheless diffuse everywhere. However, if some regions of the ratchet surface reflect specularly and others diffusely, the non-equilibrium velocity distribution can be exploited for momentum transfer in the tangential direction [7], this mechanism resides in the symmetry-breaking of surface reflection behaviours [8]. In this way, it is possible to convert thermal energy into mechanical energy in this structure [7]. The inclined specular surface serves as a rectifier transferring momentum onto the upper wall. The energetic performance of this engine has been investigated in the free molecular [7] and transition regime [9], and for a given configuration the maximal power output is found to be reached
in the transition regime. Previous analysis on this engine reveals low efficiency in the free molecular regime [7], and the efficiency is even lower when the specular surface is vertically placed [9], whereas the influence of the inclination angle on the thermodynamic performance of this engine has not been explored.

In the transition regime, the Navier-Stokes-Fourier (NSF) equations are no longer applicable, whereas one must resort to the Boltzmann equation [1, 10, 11]. The direct simulation Monte Carlo (DSMC) method is computationally expensive in this regime due to the explicit decoupling of molecular movement and collision steps [12]. Recently an alternate approximation to the Boltzmann equation by a Fokker-Planck (FP) model has been shown to be computationally more attractive than DSMC [13–17]. The Fokker-Planck model replaces the Boltzmann collision operator with a Fokker-Planck operator consisting of a drift term and a diffusive term. In this sense, the molecular velocity is treated as a continuous stochastic process, and the corresponding evolution can be described using Langevin simulation. This releases the restriction on explicitly resolving the binary collisions in the DSMC procedure. Therefore the particle Langevin simulation is more efficient than DSMC for simulating gas flows in the transition regime.

However, some issues exist with the transport coefficients predicted by the original FP model [13], more specifically, the Prandtl number \( Pr = \frac{\nu}{\kappa} \) is incorrect for monatomic gases, where \( \nu \) and \( \kappa \) are the viscosity and thermal conductivity coefficients, respectively. Later works manage to tackle this critical issue by modifying the drift term [16] or the diffusive term [18] in the FP model, such that the correct \( Pr = 2/3 \) is obtained. It deserves to mention that on the theoretical side, the ESFP model has been shown to give the correct Prandtl number, and the H-theorem is respected. In this study, for the numerical simulation of ratchet channel gas flow, we employ the ellipsoidal statistical Fokker-Planck (ESFP) model proposed in Ref [18], along with the numerical integration scheme for the Langevin simulation developed in Ref [19].

In this work, we perform numerical simulation for the ratchet channel nonequilibrium gas flows in the transition regime. The thermal efficiency is optimized with respect to the moving wall velocity and the inclining angle of the specular wall, and the maximal efficiency optimized with respect to the inclination angle is found to be not much different from that in the free molecular regime.

This paper is organized as follows. In Section 2, we describe the ESFP model and its numerical algorithm. In Section 3, we present the simulation results and analyses. Conclusions and future perspectives are given in Section 4.

![Figure 1](image_url) Figure 1. (a) Periodically structured two dimensional microchannel with the top and bottom surface held at constant temperatures \( T_1 \) and \( T_2 \), respectively. (b) Single unit cell of ratchet channel. The dotted (solid) lines denote the diffusely (specularly) reflecting wall.

2. The governing equation

The evolution of the molecular density function \( \mathcal{F} \) in the \( x-V \) space is governed by the Boltzmann equation with the Fokker-Planck operator [18, 19]

\[
\frac{\partial \mathcal{F}}{\partial t} + V_i \frac{\partial \mathcal{F}}{\partial x_i} = -\frac{\partial (A_i \mathcal{F})}{\partial V_i} + \frac{1}{2} \frac{\partial^2 (D_{ij} \mathcal{F})}{\partial V_i \partial V_j}
\]
where the right hand side term, in its most general form, contains a drift coefficient $A_i$ and a diffusion coefficient tensor $D_{ij}$. Note that Einstein’s summation convention is adopted hereafter. In the original model proposed by Jenny [13], the diffusion tensor is diagonal, i.e., $D_{ij} = \delta_{ij}RT/\tau$ while the ESFP model employed in this paper is anisotropic, which is exploited to facilitate the correction of Prandtl number. In both cases, the drift coefficients take the same form, i.e., $A_i = -(c_i - U_i)/\tau$ where $c$ is the molecular velocity, $U$ is the stream velocity, and $\tau$ is the relaxation time.

In the ESFP model [19], the tensor $D_{ij}$ is made dimensionless by $RT$ and $\tau$, i.e., $D_{ij} = \eta_D \delta_{ij}RT/\tau$, where $T$ is the local temperature and the dimensionless tensor takes the form $E_{ij} = (1 - \nu)\delta_{ij} + \nu P_{ij}$, where $P_{ij}$ is the pressure tensor and $\nu = P_{ii}/3$ is the pressure. Here an additional parameter $\nu$ is introduced by [18] to adjust the Prandtl number, i.e., $Pr = 3/[2(1 - \nu)]$. Note that the Prandtl number makes sense only when the flow is close to the equilibrium [10], and the non-equilibrium intensity can be characterized by the eigenvalues of $P_{ij}/\rho$. In the definition of $D_{ij}$, one must ensure its positive definiteness, hence the following restriction on $\nu$ is given in [18]

$$\nu = \max\left(-\frac{5}{4}, -\frac{RT}{\lambda_{max} - RT}\right)$$  \hspace{1cm} (2)

where $\lambda_{max}$ is the maximum eigenvalue of $P_{ij}/\rho$. Note that the correct Prandtl number for monatomic gases can be recovered when $\nu = 5/4$, and the case of $\nu \neq 5/4$ corresponds to non-equilibrium flow with strong directional anisotropy.

The definition of relaxation time in the ESFP model is given by

$$\tau(t, x) = 2(1 - \nu)\mu(t, x)/p(t, x)$$  \hspace{1cm} (3)

where both the viscosity and pressure are both space-time dependent. Besides the computational part, the ESFP model also fulfils the H-theorem and the accordingly second law of thermodynamics, which has not been proven for the cubic FP model [16]. For more details and proofs of the ESFP model, we refer to the original work of Ref [18].

2.1. The particle Fokker-Planck algorithm

The particle simulation of ESFP model relies on the equivalence of the Fokker-Planck equation of a continuous stochastic process and its corresponding Langevin equation [20]. The particles evolve along individual stochastic paths subjected to the drift force and diffusive force in equation (1), the corresponding stochastic ordinary differential equation reads as

$$\dot{x}_i = c_i \hspace{1cm} (4)$$

$$\dot{c}_i = -\frac{1}{\tau}(c_i - U_i) + \sqrt{\frac{2k_BT}{m\tau}}L_{ij}\dot{W}_j \hspace{1cm} (5)$$

where $W(t)$ is a 3D Wiener process satisfying $\langle \dot{W}_i(t) \rangle = 0$ and $\langle \dot{W}_i(t)\dot{W}_i(t') \rangle = \delta_{ij}\delta(t - t')$. The matrix $L$ is the Cholesky decomposition of matrix $E$, i.e., $L^TL = E$. For the time discretization of equations (4) and (5), an exact integration scheme has been proposed in Ref [19], which is written in the discretized form

$$c_i^{n+1} = U_i^n + (c_i^n - U_i^n)e^{-\Delta t/\tau} + \sqrt{\sigma_{cc}^2/\sigma_{xx} L_{ij}\xi_j} + \sqrt{\sigma_{cc}^2 - \sigma_{cx}^2/\sigma_{xx} L_{ij}\eta_j} \hspace{1cm} (6)$$

$$x_i^{n+1} = x_i^n + U_i^n\Delta t + (c_i^n - U_i^n)(1 - e^{-\Delta t/\tau})\tau + \sqrt{\sigma_{xx} L_{ij}\xi_j} \hspace{1cm} (7)$$

where $\xi = (\xi_1, \xi_2, \xi_3)$ and $\eta = (\eta_1, \eta_2, \eta_3)$ are independent random vectors with each component sampled from standard normal distribution, and the coefficients are

$$\sigma_{cc} = RT(1 - e^{-2\Delta t/\tau}), \quad \sigma_{cx} = \tau RT(1 - e^{-\Delta t/\tau})^2, \quad \sigma_{xx} = \tau^2 RT(2\Delta t/\tau - 3 + 4e^{-\Delta t/\tau} - e^{-2\Delta t/\tau}) \hspace{1cm} (8)$$

Here we use a simpler position updating scheme, i.e., $x_i^{n+1} = x_i^n + U_i^n\Delta t$, for the sake of computational efficiency. This position update scheme has been previously used in the cubic FP model [14, 16].
2.2. Macroscopic fields evaluation
For the evaluation of flow field quantities, i.e.

\[ P(x, t) = \int \mathcal{F}(x, V)Q(V)\,dV \]  

(9)

Assume \( n_p \) simulation particles reside in a cell at location \( x \), the field quantity can be approximated as

\[ P(x, t) = \frac{1}{dV} \sum_{k=1}^{n_p} Q(e^k(t))w_k \]  

(10)

where \( dV \) is the cell volume, \( w_k \) represents the weight of a number of molecules. In order to obtain the statistically stationary solution, one uses time averaging to evaluate the moments

\[ P^{n+1}(x) = \left(1 - \frac{1}{n}\right) P^n(x) + \frac{1}{n} \frac{1}{dV} \sum_{k=1}^{n_p} Q(e^k(t))w_k \]  

(11)

where \( n \) denotes the time step. Note that the purpose of calculation of moments is twofold: first, calculating the drift and diffusion terms and second, obtaining the flow fields quantities.

Table 1. Outline of the ESFP algorithm.

| Step | Description |
|------|-------------|
| 1.   | Initialise the particles position and velocity. |
| 2.   | Move the particles according to equation (7). |
| 3.   | Apply the wall boundary conditions similar to DSMC. |
| 4.   | Calculate the moments in each computational cell according to equation (10). |
| 5.   | Update the particle velocities according to equation (6). |
| 6.   | Sample the flow fields using equation (11). |

3. Simulation of Ratchet Channel Gas Flow
The ESFP algorithm is outlined in Table 1. The simulation is conducted in a unit cell of as shown in Fig 1(b). The top boundary is diffusive everywhere and it has uniform temperature \( T_1 = 273K \). The bottom boundary is composed of specularly and diffusively reflecting surfaces, both being held at constant temperature \( T_2 = 573K \). The specular surface is tilted with an inclination angle. The top wall is allowed to slide horizontally for the purpose of energy conversion.

The ESFP code we developed here is basically adapted from the open source OpenFOAM solver dsmcFoam, which is inherited from the particle and cloud libraries. The channel is discretized with structured mesh using the OpenFOAM meshing utility blockMesh. Initially, the number density of each cell is specified according to a linearly varying temperature in the y direction of the channel. On average each cell is equipped with 80 simulation particles initially. The solver was run with 8 message passing interface (MPI) processors on a CPU-Intel (R) @ 3.60 GHz, and typically the overall computation time was about 20 hours when the steady solution is reached. Note that the grid resolution is dependent on the gradients of flow field quantities and the time step size must satisfy the Courant criterion.

We fix the Knudsen number \( Kn = 0.1 \) and the geometric ratio \( H/L = 0.3 \) and \( B/L = 0.3 \), hence the relevant parameters are the inclination angle and the moving velocity \( \bar{U}_w = U_w/\sqrt{2RT_1} \). For the case of \( \alpha = 20^\circ \) and various values of \( \bar{U}_w \), the shear stress and heat flux is plotted along the upper wall as depicted in figure 2(a) and figure 2(b), respectively. Note that in this case the shear force acting on the upper wall is always positive, which facilitates the enhancement of the mechanical power and thermodynamic efficiency of this engine. Note also that the statistical scatter is comparable to that presented in [9] using DSMC, but the computation time is relatively smaller, which comes at the price of increasing the number of particles and samples used for time averaging in equation (11).

The propelling force decreases with the wall velocity as exhibited in figure 2 (a), which results in a maximum of the work output with respect to the wall velocity. This fact is reflected in the efficiency \( \eta = U_w F_{xy}/Q_y \) as shown in figure 2(c), where the total heat flux and the force are obtained by
integrating \( q_y \) and \( \sigma_{xy} \) over the upper wall. Note that the maximum efficiency is achieved at about \( \bar{U}_w = 0.04 \), which is close to that predicted in the free molecular regime [7].

![Figure 2](image)

Figure 2. (a) Dimensionless shear stress \( (\bar{\sigma}_{xy} = \sigma_{xy}/(\rho RT)) \) distribution along the upper wall for various values of \( \bar{U}_w \). (b) Dimensionless heat flux \( (\bar{q}_y = q_y/(\rho(2RT)^{3/2})) \) distribution along the upper wall for various values of \( \bar{U}_w \). (c) Efficiency as a function of wall velocity for \( \alpha = 20^\circ \). (d) Efficiency as a function of inclination angle for \( \bar{U}_w = 0.04 \).

For fixed \( \bar{U}_w = 0.04 \) we calculate the efficiency as a function of the angle as shown in figure 2(d). This strong dependence on \( \alpha \) bear resemblance to that reported in Ref [7], although the efficiency here is not optimized with regard to \( \bar{U}_w \). In this configuration, the optimal angle that maximizes the efficiency is about \( 20^\circ \), which is again close to that predicted in Ref [7]. The “flatter” (smaller \( \alpha \)) specular surface acts as a ”better” guide for particles moving from the lower diffuse wall to the upper wall such that the momentum and energy and the resulting force exerting on the upper wall becomes larger. Note that in this study the channel ratio \( B/L \) is larger than that in [7], this reduction in efficiency for a relatively larger channel width is in accordance with the observations in Ref [9].

4. Summary
In this study, we have simulated the thermally driven flow in a ratchet channel using the recently developed particle ESFP method. We investigate the mechanical power output and thermal efficiency in the transition regime when this device acts as an energy converter. Our results complement the previous analysis in the free molecular regime and numerical simulation in the transition regime for this engine. The simulation results confirm the enhanced performance with an inclined specular wall compared to a vertical one as previously reported in the literature. It is found that in the transition regime, the dependence of the efficiency on inclination angle is similar to that in the free molecular limit.
Moreover, it is expected that the ESFP model suffers from statistical noise like DSMC, especially in the case of low speed flows. To tackle this issue, one may incorporate the present ESFP model with more efficient methods such as octant flux splitting information preservation method [21], the low-variance Monte-Carlo simulation method [22], as well as the variance reduction approach with the assist of parallel correlated stochastic process [23, 24]. The efficient particle algorithm can facilitate the parameter study and optimization of ratchet gas flows.

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