Use of the degenerated Reynolds equation in solving the microchannel flow problem

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In this paper, the author proposes that the generalized Reynolds equation employed in the gas film lubrication problems, where the flow rates of the Poiseuille flow are calculated from the Boltzmann equation, can be degenerated for solving the microchannel flow problem in the transitional regime. Using this approach, the calculated results of pressure distribution in long microchannels show excellent agreement with the experimental data and the result of the information preservation (IP) method. The results in short microchannels show excellent agreement with the direct simulation Monte Carlo method and the IP method. The lattice Boltzmann method solution of the microchannel flow is examined by comparison with the degenerated Reynolds equation calculations and the disagreement in the pressure distribution confirms that the lattice Boltzmann method is unsuitable for the solution of the microelectromechanical systems (MEMS) flows in transitional regime. For microchannel flows, the degenerated Reynolds equation can serve as a criterion having the merits of kinetic theory for testing various methods intending to solve rarefied gas flow problems in MEMS devices in the transitional flow regime. © *2005 American Institute of Physics*.
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I. INTRODUCTION

Since the 1990s, the micromachining technologies for the fabrication of microsystems have become more and more mature. Based on these techniques, the microelectromechanical systems (MEMS) developed rapidly and found many applications not only in microelectronics, but also in medicine, biology, optics, aerospace, and other high technology fields. Both experimental and computational efforts have been undertaken to understand the specific features of the microscale flows. Microchannel is a basic constituent of the MEMS devices, its geometric form is regular and simple (see Fig. 1), but it can reveal many specific features of the low speed microinternal flows. The UCLA–Caltech researchers first proposed and fabricated an integrated microchannel/pressure sensor system using the combined surface bulk silicon micromachining.[1,2] The second generation microchannel[2] is 40 μm wide and 1.2 μm high with 11 pressure sensors uniformly distributed along the 4000 μm length of the channel at intervals of 400 μm. The Knudsen number at the outlet of the channel under STP is $\sim$0.055 for nitrogen and is $\sim$0.16 for helium, the flow is surely beyond the slip flow regime. The MIT microchannels[3,4] were fabricated in almost the same way with a height of 1.33, width 52.25, and length 7500 μm. Nitrogen, argon, carbon dioxide, and helium have been used as the working media, the flow of argon has a Knudsen number of 0.05 at the exit at atmospheric pressure and that of helium has a Kn$\sim$2.5 at the exit at a low pressure of 6.5×10^3 Pa. The pressure distribution along the channel and the flow rates through the channel were measured and the pressure distribution was found to deviate from the linear distribution of the Poiseuille flow and the experimental results were compared only with the slip Navier–Stokes equation solution,[1–4] while the flow was certainly in the transitional regime. Utilization of direct simulation Monte Carlo (DSMC) method[5] in simulating microchannel flows is appropriate but it has the problems of the excessively high demands on storage capacity and computation time. The necessary gradual regulation of the inlet and outlet boundary conditions of low speed flow in the channel seems to be tremendously difficult for DSMC in solving the long channel problems. Up to the present the DSMC simulation of the microchannel flow has been limited to very short channels or to the high speed and even hypersonic cases.[6,7] Recently, Shen, Fan, and Xie[8] successfully simulated the microchannel flows under the experimental conditions[1–4] using the information preservation (IP) method[9,10] by the employment of the conservative scheme and superrelaxation technique, with results in excellent agreement with the experimental data.[1–4] Still it is desirable to have a direct test by a test stone with the merits of kinetic theory to verify the IP method. The author proposes that the generalized Reynolds equation for calculating the gas film lubrication problem, where the flow rates of the Poiseuille flow are calculated from the linearized Boltzmann equation,[11] can be degenerated for the solution of the microchannel flow problem. In the following the generalized Reynolds equation is briefly introduced and its results in calculating the gas film bearing are compared with the DSMC and IP calculations. Then it is shown how the degeneration of the Reynolds equation is used to solve the microchannel problem. Comparison of the calculations of the microchannel flows by the degenerated Reynolds equation with the experimental results and the simulation results of the IP

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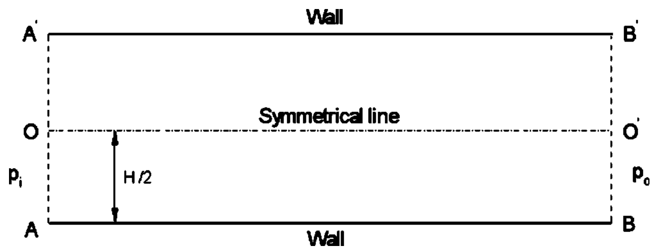

FIG. 1. Schematic of the microchannel flow.

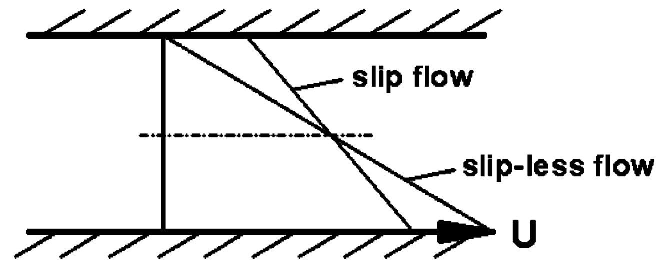

FIG. 3. Velocity profiles and the flow rates of the slip-less and slip Couette flow.

and DSMC methods shows excellent agreement. The lattice Boltzmann method (LBM) solution of the microchannel flow has been compared earlier with the DSMC and IP calculations but in this paper it is reexamined by comparison with the degenerated Reynolds equation calculations and the disagreement in the pressure distribution reveals again that the lattice Boltzmann method is unsuitable for solving the MEMS flows in the transitional regime.

II. THE GENERALIZED REYNOLDS EQUATION

The squeezed air bearing problem in the Winchester-type hard disk drive may be schematically modeled as a lower plate (the surface of the spinning platter) moving in its own plane with a velocity of U under the upper stationary tilted plate (the read/write head, see Fig. 2). The thin film air flow between the plates is most appropriately described by the Reynolds equation which is an integrated mass conservation relationship applied to a cross section of the gap of height h between the plates at position x relating the pressure p, density ρ, platter velocity U, and the height h of the gap, first developed by Reynolds for continuum fluid.[12] It is a mass conservation relation applied not to a fluid element but to a cross section of the squeezed air flow and is obtained from the continuity equation by integrating it over the vertical direction from the lower plate to the upper plate with the employment of the momentum conservation equation. By introducing $X=x/L$, $H=h/h_o$, $P=p/p_o$, and the bearing number $\Lambda=6\mu UL/p_o h_o^2$, the Reynolds equation for the steady and two-dimensional case can be written in the normalized form[13]

$$\frac{d}{dX}\left(H^3 P\frac{dP}{dX}\right)=\Lambda\frac{d}{dX}(PH). \tag{1}$$

This equation shows that the flow rate through any cross section is the sum of the flow rates of the Couette flow (the right-hand side) and the Poiseuille flow (the left-hand side with the negative sign) and this rate does not change from one cross section to another in steady flow. Equation (1) is extended to the slip flow case by Burgdorfer.[14] From the solution of the simple slip flow problem it is known that the flow rates of the Poiseuille flow with slip boundary condition surpasses that of the slip-less case by a factor (see, e.g., Ref. 15) of

$$\frac{Q_{P,SL}}{Q_{P,C}}=\left(1+6\frac{2-\sigma}{\sigma}\mathrm{Kn}\right), \tag{2}$$

where σ is the tangential accommodation coefficient. For the Couette flow the flow rates have a specific feature, i.e., they are identical in the slip-less case and the slip case (and even in the transitional regime case) and have the following value independent of the Knudsen number owing to the symmetry of the flow (see Fig. 3):

$$Q_C=\rho Uh/2. \tag{3}$$

So the following Reynolds equation is obtained in the slip flow regime in place of Eq. (1):

$$\frac{d}{dX}\left[\left(1+6\frac{2-\sigma}{\sigma}\mathrm{Kn}\right)H^3 P\frac{dP}{dX}\right]=\Lambda\frac{d}{dx}(PH), \tag{4}$$

where $\mathrm{Kn}=\lambda/h$ is the local Knudsen number. Fukui and Kaneko[11] showed that the solution of the linearized Boltzmann equation for the thin film bearing problem can be decomposed into the solutions of the plane Couette flow and the plane Poiseuille flow.[16] On this basis they derived the generalized Reynolds equation for the thin film air bearing problem by employing the flow rates of the fundamental Poiseuille and Couette flows solved by the linearized Boltzmann equation. This generalized Reynolds equation in the isothermal case can be written as[11]

$$\frac{d}{dX}\left[\overline{Q}_{P,TR}(\mathrm{Kn})H^3 P\frac{dP}{dX}\right]=\Lambda\frac{d}{dx}(PH), \tag{5}$$

where $\overline{Q}_{P,TR}(\mathrm{Kn})$ is the flow rate in the transitional regime (normalized by the slip-less value $Q_{P,C}$) calculated from the linearized Boltzmann equation for Poiseuille flow and is shown to be the same as that solved by Cercignani and Daneri.[16] A table database of the calculated values of $\overline{Q}_{P,TR}(\mathrm{Kn})$ for $\sigma=1$, $\sigma=0.9$, $\sigma=0.8$, and $\sigma=0.7$ is provided in Ref. 17, and a fitted formula approximation for diffuse reflection ($\sigma=1$) by Robert is recorded in Ref. 18,

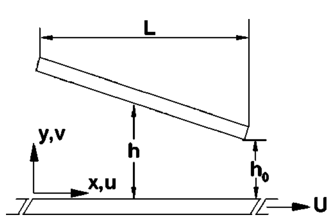

FIG. 2. A schematic model of the thin film air bearing flow.

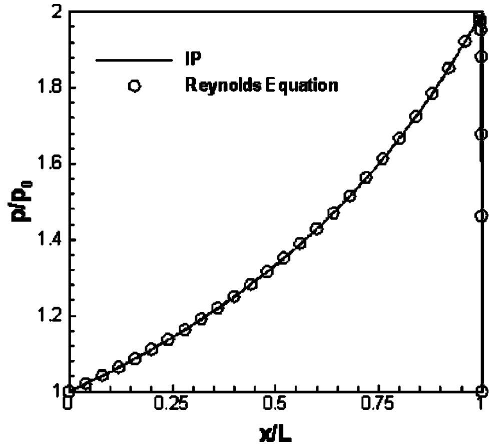

FIG. 4. Pressure distribution in the actual length disk driver bearing for $\mathrm{Kn}_o=1.25$, $L=1000$ μm, comparison of IP method (solid line), and the generalized Reynolds equation results (Ref. 19) (circles).

$$\overline{Q}_{P,TR}(\mathrm{Kn}) = 1 + 6A\mathrm{Kn} + \frac{12}{\pi}\mathrm{Kn}\ln(1 + B\mathrm{Kn}), \tag{6}$$

where $A=1.318\,889$ and $B=0.387\,361$. Alexander, Garcia, and Alder[18] used the DSMC method to simulate the short head length air bearing problem ($L=5$ μm, $h_o=50$ nm $=0.05$ μm, $U=25$ m/s, $\sigma=1$, and also with alternative similar conditions), and found excellent agreement of the DSMC simulation with the generalized Reynolds equation (5) and Eq. (6). Note, their description of the latter as continuum hydrodynamic Reynolds equation corrected for slip is misleading. As we have shown, the generalized Reynolds equation is a global mass conservation relation applied to the cross section of the air bearing flow with the flow rate calculated by the Boltzmann equation. Recently, Jiang, Shen, and Fan[19] solved the thin film air bearing problem by the IP method. Figure 4 shows the comparison of the pressure distributions for the cases of the actual length $L=1000$ μm of the read/write head calculated by the IP method and by the generalized Reynolds equation. One can see the agreement is excellent. This can be considered as a verification of the IP method used for solving a problem with significance of practical application in a test having the merits of the strict kinetic theory of gases.

III. DEGENERATION OF THE REYNOLDS EQUATION FOR SOLVING THE MICROCHANNEL FLOW

The generalized Reynolds equation (5) is originally derived for application in the thin film air bearing problem with the lower plate moving with a velocity U and the upper plate tilted. We suggest using this Reynolds equation to solve the microchannel flow problem in which the lower plate is stationary and the upper plate is parallel to the lower one. Owing to the steadiness of the lower plate the right-hand side term vanishes, as $U=0$ and $\Lambda=0$, there is not any contribution of the Couette flow. Owing to the parallelity of the two plates the value H is a constant and can be dropped from the equation. So the generalized Reynolds equation for application to the microchannel problems is degenerated to the form

$$\frac{d}{dX}\left[\overline{Q}_{P,TR}(\mathrm{Kn})P\frac{dP}{dX}\right] = 0. \tag{7}$$

The values of P at the inlet ad outlet of the channel are to be specified to make the microchannel problem solvable. This degenerated Reynolds equation is proposed by the author to be used for solving the microchannel flow in the transitional flow regime provided the flow rate of the local Poiseuille flow $\overline{Q}_{P,TR}(\mathrm{Kn})$ in transitional regime (normalized by the slip-less value $Q_{P,C}$) is known from the strict kinetic theory. There are many works devoted to the solution of the Poiseuille flow providing the database for the flow rates at different Knudsen numbers and for different boundary conditions at the surface. With the database incorporated the degenerated Reynolds equation is valid for any surface conditions of the plates and can be integrated numerically. For example, the incomplete diffuse reflection cases with tangential accommodation coefficient $\sigma=1$, $\sigma=0.9$, $\sigma=0.8$, and $\sigma=0.7$ were calculated in Ref. 17 with table database of the values of $\overline{Q}_{P,TR}(\mathrm{Kn})$ provided under these boundary conditions. If the practical case has the need, even situations with two plates having different accommodation coefficients could be considered. But for illustrative purposes only the case of completely diffuse reflection, $\sigma=1$, is expounded here. For this case the fitted formula approximation of $\overline{Q}_{P,TR}(\mathrm{Kn})$, Eq. (6), can be used, and the degenerated Reynolds equation attains the form

$$\frac{d}{dX}\left\{\left[1 + 6A\mathrm{Kn} + \frac{12}{\pi}\mathrm{Kn}\log(1 + B\mathrm{Kn})\right]P\frac{dP}{dX}\right\} = 0. \tag{8}$$

For the ease of integration the local Knudsen number Kn is most conveniently expressed through P, e.g., for hard sphere models it can be written as

$$\mathrm{Kn} = \frac{\lambda}{h} = \frac{C}{P}, \tag{9}$$

where

$$C = \frac{\mu}{p_0 h}\sqrt{\frac{\pi R T_0}{2}} = \lambda_0/h = \mathrm{Kn}_{out}, \tag{10}$$

for we have for hard sphere

$$\lambda = \frac{\mu}{p}\sqrt{\frac{\pi R T}{2}}, \tag{11}$$

and p_0 is the pressure at the outlet, T_0 is the temperature of the gas, and μ is the viscosity of the gas at T_0. The constant C has the physical meaning of the Knudsen number at the outlet of the channel [see Eqs. (9) and (10), at outlet $P=1$]. Substituting Eq. (9) into Eq. (8), one arrives at the degenerated Reynolds equation for microchannel flow with the diffuse reflecting surface

$$\left[P + 6AC + \frac{12}{\pi}C\log\left(1 + \frac{BC}{P}\right)\right]\frac{dP}{dX} = D, \tag{12}$$

where D is an unspecified constant to be determined from the integration and has the physical meaning of the flow rate through the channel normalized by the slip-less flow rate

TABLE I. The experimental inlet pressure data in psi (gauge) and corresponding values of $P|_{X=0}$ for nitrogen and helium.

			For nitrogen		
p_{in} [psi (guage)]	5	10	15	20	25
$P\|_{X=0}$	1.3402	1.6805	2.0207	2.3609	2.7012
			For helium		
p_{in} [psi (guage)]	8.7	13.6	19.0		
$P\|_{X=0}$	1.5920	1.9254	2.2929		

value. To illustrate the use of the degenerated Reynolds equation in solving the microchannel problem we calculate the pressure distribution for nitrogen in the $1.2\times 40 \times 3000\ \mu\text{m}^3$ channel[1] and helium in the $1.2\times 40 \times 4000\ \mu\text{m}$ channel.[2] For $T_0 = 294$ K the value of C for helium is 0.155 79, and for nitrogen is 0.052 325. Equation (12) is integrated under the following boundary condition:

$$P|_{X=0} = p_{in}/p_{out}, \quad P|_{X=1} = p_{out}/p_{out} = 1. \tag{13}$$

The pressures p_{in} at the inlet of the channel are taken as the experimental data in Refs. 1 and 2. The experimental values of p_{in} in psi (gauge) given in Refs. 1 and 2 and the corresponding values of $P|_{X=0}$ are listed in Table I. The results of integration are presented in Figs. 5 and 6. From these figures one sees that the agreement between the IP result and the result of the degenerated Reynolds equation is excellent, the curves for the helium case cannot be distinguished from each other, the experimental data agree with the above two methods within the limit of the experimental accuracy.

In fact the degenerated Reynolds equation is the global mass conservation equation obtained from the constancy of the flux across any cross section of the channel. This idea can be developed to obtain easily the pressure distribution along the channel in the continuum and slip flow regimes.

IV. EXAMINATION OF THE FEASIBILITY OF THE LATTICE BOLTZMANN METHOD IN SOLVING THE TRANSIONAL FLOW PROBLEM

The lattice Boltzmann method (LBM, see Ref. 20, and references cited therein) solves the simplified Boltzmann equation on lattice points. LBM solution converges to the Navier–Stokes solution for small Kn. The ease of LBM in handling complex geometry, simplicity in implementation and its high efficiency makes it tempting to use it in simulating gas flows in MEMS. Recently Nie, Doolen, and Chen[21] attempts to use it in the transitional regime. It is of fervent concern for the scientific community to know whether LBM is capable to simulate correctly the transitional regime flows in MEMS. Shen, Tian, Xie, and Fan examined the suitability of using LBM in simulating MEMS flows by comparison with the DSMC calculations.[22] Here the LBM results are compared with the calculations using the degenerated Reynolds equation and the same conclusion as in Ref. 22 is reached, but this time the conclusion is confirmed by a test stone having the merits of strict kinetic theory.

Equation (12) is integrated under the following conditions for a short $1\times 100\ \mu\text{m}^2$ microchannel that has been considered with LBM in Nie, Doolen, and Chen:[21]

$$C = 0.194, \quad P|_{X=0} = 2, \quad P|_{X=1} = 1, \tag{14}$$

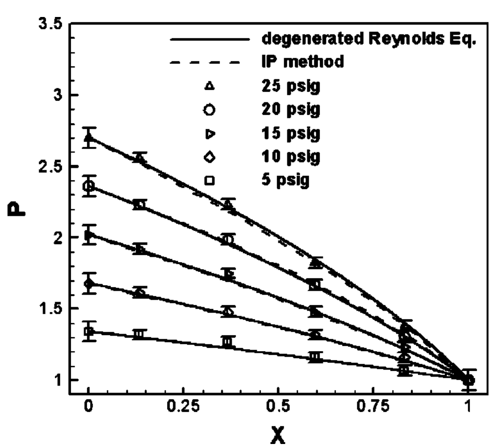

FIG. 5. The pressure distribution in a $1.2\times 40\times 3000\ \mu\text{m}^3$ microchannel for nitrogen. Comparison of the degenerated Reynolds equation (12) (solid line), the IP method (dashed line) (Ref. 8), and the experimental data (△, ○, ▷, ◇, □), the figures in the units of psi (gauge) indicate the pressures at the inlet of the channel) (Ref. 1).

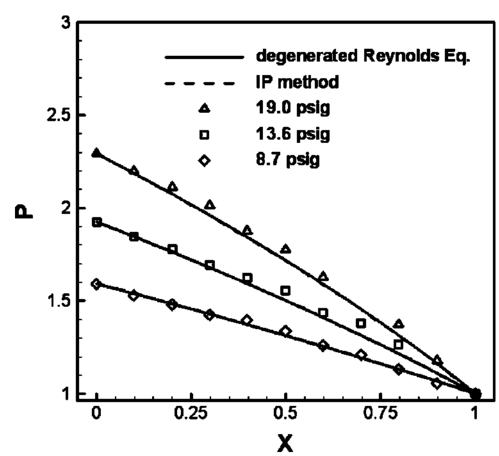

FIG. 6. The pressure distribution in a $1.2\times 40\times 4000\ \mu\text{m}^3$ microchannel for helium. Comparison of the degenerated Reynolds equation (12) (solid line), the IP method (dashed line) (Ref. 8), and the experimental data [△, □, ◇, the figures in units of psi (gauge) indicate the pressures at the inlet of the channel] (Ref. 2). It is noted that the curves for the degenerated Reynolds equation and for the IP method can hardly be distinguished from each other.

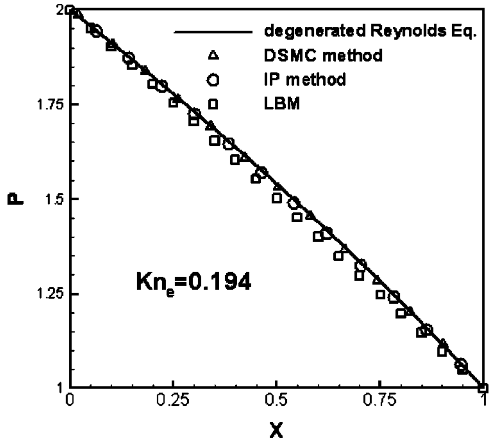

FIG. 7. The pressure distribution in a $1\times 100\ \mu m^2$ microchannel for Kn =0.194. Comparison of the degenerated Reynolds equation (12) (the solid line), the DSMC method (triangles), the IP method (Ref. 21) (circles) and the LBM method (Ref. 20) (squares).

$$C = 0.388, \quad P|_{X=0} = 2, \quad P|_{X=1} = 1. \tag{15}$$

The comparison of results of the degenerated Reynolds equation (12) with those of Nie, Doolen, and Chen by using the lattice Boltzmann method (LBM) (Ref. 21) are shown in Figs. 7 and 8. Also shown are the DSMC and IP results. From the comparison it is seen that the DSMC method, the IP method, and the degenerated Reynolds equation yield almost identical pressure distribution, but the LBM results are quite different from the calculations of the degenerated Reynolds equation and as well from DSMC and IP results, so it can be concluded that the version of LBM employed in Ref. 21 is not suitable for simulating microchannel flows in the transitional regime. For the detailed examination of the feasibility of the LBM method in simulating transitional regime microchannel flows, readers are referred to Ref. 22 where among other things the version of LBM used[21] was briefly described. Also, there the comparison of the pressure distributions was given in the form of deviation from linearity, so the differences between results of various methods were revealed in a more distinguishable way. In this paper the quantities being compared are the pressure distributions themselves and the same conclusions are achieved (see Figs. 7 and 8). But here the conclusion is reconfirmed by the comparison with calculations having the merits of strict kinetic theory.

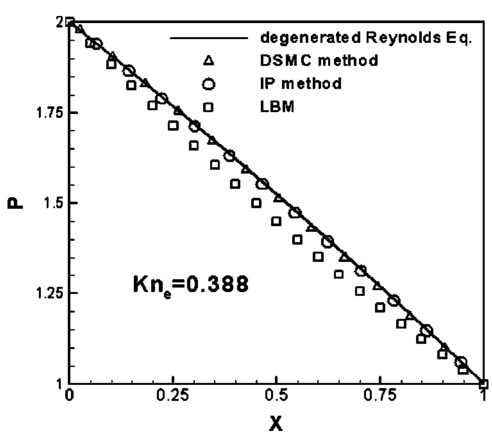

FIG. 8. The pressure distribution in a $1\times 100\ \mu m^2$ microchannel for Kn =0.388. Comparison of the degenerated Reynolds equation (12) (the solid line), the DSMC method (triangles), the IP method (Ref. 21) (circles), and the LBM method (Ref. 20) (squares).

It is essential to note that besides the air bearing problem and the microchannel flow problem the Reynolds equation can also model the gas damping problem in micromechanical accelerometers,[23] so the calculation of the flow rates of Poiseuille flow based on rigorous kinetic theory with practically encountered boundary conditions is actual in many practical applications.

V. CONCLUDING REMARKS

In the present paper the generalized Reynolds equation for a hard disk drive gas film lubrication problem with flow rate of the Poiseuille flow calculated from the linearized Boltzmann equation is degenerated for solving the rarefied gas flow problems in microchannels. The results show excellent agreement with the experimental data and the IP results in the long microchannels. Before this the IP results for long channel have only been compared with the experimental data (the DSMC was not able to accomplish simulation of the long channel flow where the experimental data were available), now they are verified by comparison with results of the degenerated Reynolds equation. This is a verification of the IP method for the two-dimensional case having direct significance in practical application by a method based on kinetic theory. With the degenerated Reynolds equation in hand we have a means with the merit of strict kinetic theory to test various methods intending to solve the microscale rarefied gas dynamic flows in transitional regime. The unsuitability of LBM for solving the transitional flow problem was shown before by comparison with the DSMC results, now this conclusion is reconfirmed by comparison with the degenerated Reynolds equation. From the practical application viewpoint, creating a database for the flow rates of the Poiseuille flow with various combinations of possible surface properties calculated on the basis of Boltzmann equation or other strict kinetic theory is an actual task for the solution of the microchannel flow, the thin film air bearing problem and also the gas damping problem in micromechanical accelerometers. The database in the form of fitting formulas is especially desirable.

ACKNOWLEDGMENTS

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