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در هفدهمین کنفرانس دینامیک شاره‌ها که از تاریخ ۵ تا ۷ شهریور ماه ۱۳۹۶ در

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A THOROUGH EVALUATION OF THE FOKKER-PLANCK KINETIC MODEL IN THE COUETTE FLOW

ارائه نموده‌اند.

دکتر محمد حسن کیهانی
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برگزار کنندگان



کمیته برگزاری

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Abstract

In this paper, the evolution of Fokker-Planck (FP) approach in various Knudsen numbers and number of particles per cells (PPC) was investigated. A canonical argon Couette flow has been chosen. However, there are some other direct simulation approaches to model rarefied gases such as DSMC and Lattice Boltzmann; Ideally, one would like to have an accuracy of DSMC method with computational efficiency of mesoscale methods such as LB. In this paper, it was pointed out that another possible computationally attractive option is to work with the Fokker-Planck kinetic model. The results show that this method is acceptable up to moderate Knudsen ranges. Additionally, with about 1000 PPC the computational efficiency is really approximate in comparison with DSMC. Also, the dependence of FP method to the computational grid is lower than other approaches. Therefore, this method can be work with a few computational grids. However, the Fokker Planck model was used and was developed; there is no evaluation and validation due to cell, PPC and time step.

Keywords: Fokker-Planck kinetic model, Knudsen number, kinetic theory, Boltzmann equation, Particles per cells.

1. Introduction

Rarefied gas flows are present in many mechanical and aerospace systems and physical phenomena; ranging from satellite controllers and solar winds to gas separation mechanisms, micro-electro-mechanical systems (MEMS) and NEMS. Navier-Stokes-Fourier equations fail to describe gas flow in these applications accurately. This makes the modeling of rarefied gas flows a vital issue in engineering sciences.

One of the most successful numerical methods for rarefied gas flow simulations is direct simulation Monte Carlo (DSMC), which is based on the Boltzmann equation. However, the DSMC performance is not very satisfactory for near continuum and continuum regions .

Different modeling attempts were made in order to simplify the complex Boltzmann governing equation¹⁻⁴. One candidate is the Fokker-Planck equation. Fokker-Planck kinetic model based on the Boltzmann equation is considered for near continuum problems⁵.

In domains of small to moderate rarefaction (length scales greater than the mean free path), the Fokker-Planck equation furnishes a good macroscopic model of overall particle advection and diffusion that can operate on much larger length and time scales⁵.

The Fokker-Planck approximation of the Boltzmann equation can be used for rarefied gas flows as shown in many previous works. The objective of this model is the numerical advantage because the resulting diffusion model is computationally less challenging than the Boltzmann collision integral. A particle Monte Carlo scheme based on the Fokker-Planck equation was proposed by Gorji et al⁶. and was later extended to the cubic model to honor the decent Prandtl number for a monatomic gas. It should be mentioned that other researchers have also developed solution algorithms based on the Fokker-Planck model.

The cubic FP model considered in this article provides an evolution equation for the distribution function. The model is constructed such that it gives rise to correct viscosity and heat conductivity coefficients at the hydrodynamic limit, as well as an accurate description of macroscopic flow properties for the non-equilibrium condition⁷.

Note that the cost of the FP solution is independent of the Knudsen number since no collisions are computed. Moreover, time steps larger than the mean collision time and grid spacings greater than the mean free path are allowed. At the same time, accurate descriptions of rarefied gas flow can be obtained for a considerable range of Knudsen numbers⁸.

In this paper, cubic Fokker-Planck model was discussed due to change of particles per cell, number of cells and Knudsen number.

2. Fokker-Planck approximation of the Boltzmann equation

Consider the Boltzmann equation as described below:

$$\left(\frac{\partial F}{\partial t}\right)_{coll} = \frac{1}{m} \int_0^{4\pi} \int_{R^3} (F(V^*)F(V_1^*) - F(V)F(V_1)) g \sigma(\Omega, g) d\Omega d^3V_1 \quad (1)$$

If the Knudsen number is not too large, the temporal derivative of F can be approximated by the Fokker-Planck equation:

$$\left(\frac{\partial F}{\partial t}\right)_{coll} \approx -\frac{\partial}{\partial V_i} (A_i F) + \frac{1}{2} \frac{\partial^2}{\partial V_i \partial V_i} (D^2 F) = S^{FP} \quad (2)$$

Here A represents drift coefficient and D accounts for the positive diffusion which are functions of F .

relaxation of higher order moments can be controlled by appropriate expressions of A_i as polynomial functions of V_i . This leads to a set of macroscopic moment equations with physically correct macroscopic coefficients like viscosity μ and the Prandtl number Pr ⁸.

The physical assumptions implied by the FP model are⁸:

1. The particle velocities change due to a permanent stochastic force and not due to discrete collisions.

2. Particle interaction occurs due to coupling through the coefficients in the evolution equations, which are functions of stochastic moments of the local ensemble.
3. Considering the extreme case of infinite Knudsen number, i.e. no inter-molecular collisions occur, S^{FP} becomes zero, and thus the FP and DSMC models become identical.
4. In the other extreme case of extremely small Knudsen numbers, the Navier–Stokes equations are recovered by both the FP model and DSMC; the only concern here is the consistency of the macroscopic coefficients.

2.1. Coefficients

Drift and diffusion coefficients A_i and D can be derived from known velocity moment evolutions as described below. First, the velocity moments in the kinetic framework are defined. Following the same procedure for the S^{FP} operator:⁷

$$p_{ij} = -\int_{R^3} (A_i v'_j + A_j v'_i + D \delta_{ij}) F dV \quad (3)$$

$$p_i = -\int_{R^3} (A_i v'_j v'_j + 2A_j v'_j v'_i) F dV \quad (4)$$

Now the coefficients A_i and D must be found. For the drift coefficient, a quadratic polynomial function of the fluctuating velocity is presented, which honors consistent viscosity and Prandtl numbers. The simplest form of the drift coefficient is quadratic and therefore⁷:

$$A_i = \tilde{c}_{ij} v'_j + \gamma_i (v'_j v'_j - \overline{u'_j u'_j}) + \Lambda (v'_i v'_k v'_k - \overline{u'_i u'_k u'_k}) \quad (5)$$

Whereas the symmetric tensor \tilde{c}_{ij} and Λ are:

$$\tilde{c}_{ij} = -\frac{\delta_{ij}}{\tau} + c_{ij} \quad (6)$$

$$\Lambda = -\frac{1}{\alpha \rho^3} |\det(\pi_{ij})| \quad (7)$$

Where $\det(\pi_{ij})$ is determinant of the stress tensor π_{ij} and $\alpha = \tau(3kT/m)^4$ is a scaling factor with $\tau = 2\mu/p$ the relaxation time.

The simple diffusion of Langevin equation was chosen⁵:

$$D = \sqrt{\frac{4e_s}{3\tau}} \quad (8)$$

The final Fokker-Planck approximation of the Boltzmann equation for monatomic gas is derived as:

$$\frac{\partial F}{\partial t} + V_i \frac{\partial F}{\partial x_i} + G_i \frac{\partial F}{\partial V_i} + \frac{\partial \left(\left(\tilde{c}_{ij} v'_j + \gamma_i (v'_j v'_j - \overline{u'_j u'_j}) \right) + \Lambda (v'_i v'_k v'_k - u'_i \overline{u'_k u'_k}) \right) F}{\partial V_i} = \frac{\partial^2}{\partial V_j \partial V_j} \left(\frac{2e_s}{3\tau} F \right) \quad (9)$$

Whereas the coefficients \tilde{c}_{ij} and γ_i have to be determined by solving the system consisting of the linear equations¹⁰.

Although in order to derive the Fokker-Planck equation some simplifications have been made, still the high dimensionality of the solution domain makes the direct simulation of Eq. (2) rather expensive. In order to cope with that, similar to Jenny et al. 2010 the equivalent Ito processes for $M(t)$ and $X(t)$ was used^{9,11}:

$$dM_i = A_i dt + G_i dt + DdW_i \quad (10)$$

$$dX_i = M_i dt \quad (11)$$

, where dW_i is the increment of the Wiener process with zero expectation and variance dt . The physical assumptions implied by a system of equations (10) -(11) (and thus the FP model) are that the particle velocities change due to a permanent stochastic force and not due to discrete collisions. Therefore, particle interaction occurs due to coupling through the coefficients in the evolution equations, which are functions of stochastic moments of the local ensemble.¹²

A numerical scheme was considered and after discretizing equations (10) and (11) the final evolution of velocity equation and position was carried out⁸:

$$M_i^{n+1} = M_i^n + M_i^n \left(e^{-\Delta t/\tau} - 1 \right) + \sqrt{\tilde{A} - \frac{C^2}{B}} \xi_{i,u} + \sqrt{\frac{C^2}{B}} \xi_{i,x} + \frac{\Delta t}{\tau} N_i^n + G_i^n \Delta t \quad (12)$$

$$X_i^{n+1} = X_i^n + M_i^n \tau \left(1 - e^{-\Delta t/\tau} \right) + \sqrt{B} \xi_{i,x} + U_i \Delta t + \frac{\Delta t^2}{2\tau} N_i^n + G_i^n \frac{\Delta t^2}{2} \quad (13)$$

2.2. Solution algorithm

The solution algorithm that Fokker-Planck uses is⁷:

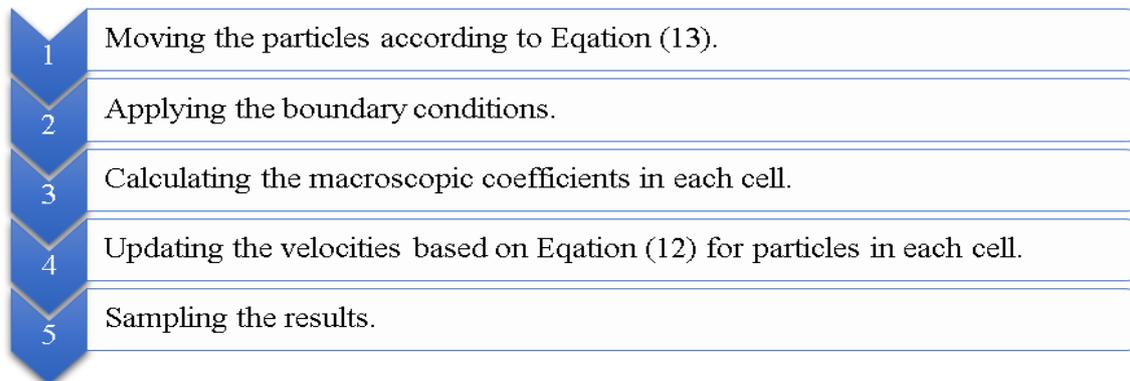


Figure 1: Fokker Planck solution algorithm

2.3. Results and discussion

In this paper, Couette flow and Fourier heat conduction were selected for verification, case study and grid independence, particle per cell (PPC) independence, Knudsen comparison and time step comparison between Fokker-Planck, DSMC, and analytical solution.

2.3.1. Couette flow

In this paper, one of the problems which was chosen to be simulated was the Couette flow. The problem considers flow inside a planar channel with parallel movement of the walls. Assuming infinitely long walls, the flow field became one dimensional. Figure 2 shows the schematic diagram of Couette flow.

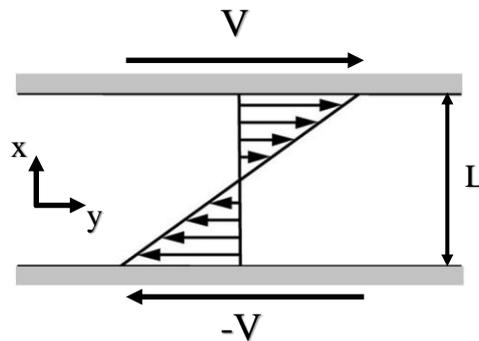


Figure 2: A schematic diagram of Couette flow

In this paper, a simple planar Couette flow of Argon was considered, and gas molecules were regarded as Maxwellian molecules with viscosity power index of 1. Walls move with a velocity of $U_{wall} = 50 \text{ m/s}$ in opposite directions, and both walls are isothermal with $T_{wall} = 273.15 \text{ K}$ and reference temperature is 273.15 K . As using cubic Fokker-Planck model the flow Prandtl number is $2/3$ which is a correct Prandtl number. Molecular mass of Argon is $6.63 \times 10^{-26} \text{ Kg}$ and molecular diameter is $4.17 \times 10^{-10} \text{ m}$.

2.3.2. Grid comparison

Figure 3 shows the grid comparison between different grids of Fokker-Planck and a DSMC grid as a benchmark. According to this figure, it is entirely clear that Fokker-Planck is not very sensitive to cell size. Also using large cell size, the results are almost accurate and near DSMC results. As 100 cells and 200 cells are very close to each other, for more precise results and further actions 100-cell grid was chosen.

As is shown in figure 3, one of the most significant advantages of the Fokker-Planck method is that it is not sensibly dependent to the grid size.

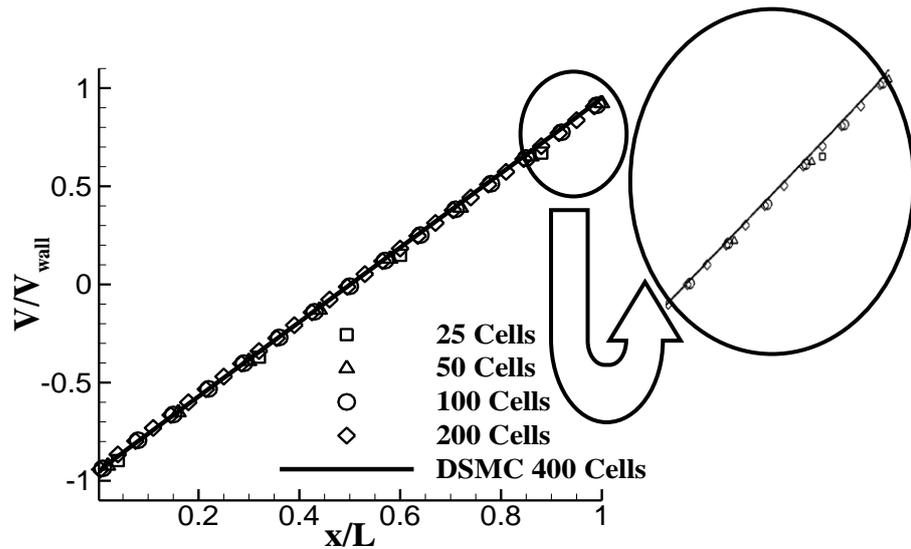


Figure 3: Grid comparison of Couette flow

2.3.3. Particle number comparison

In this section, number of particles per cell (PPC) have been investigated. Again, a simple planar Couette flow of Argon with 100 cells was chosen which is a suitable grid as mentioned in the previous section. Wall velocities are 50 m/s in opposite directions, and wall temperature is 273.15 K for all different PPCs.

For more accurate comparison between number of particles per cells, the temperature profile of Couette flow was plotted. A number of 500, 1000 and 1500 PPCs was chosen for PPC independence. As figure 4 shows 1000 PPC and 1500 PPC are very close thus 1000 PPC was selected for further comparisons. On the other hand, as illustrated in figure 4, there is a slight difference between DSMC and Fokker-Planck. The reason backs to temperature calculation of two methods.

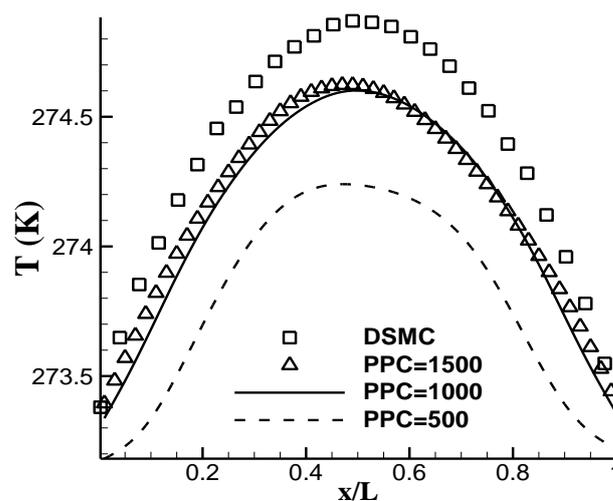


Figure 4: PPC comparison of Couette flow

2.3.4. Time step comparison

In this section, time step effect was investigated on Couette flow. Time step is defined as:

$$dt_0 = 0.5 \times \frac{\Delta x}{\sqrt{\frac{KT_{in}}{m}}} \quad (25)$$

Where T_{in} is the stream temperature. The dt_0 is the proposed referenced time step we use for Couette flow. Other time steps are selected as a fraction of this time step. For this reason, a lower time step $0.1 \times dt_0$ and two larger time steps $10 \times dt_0$ and $100 \times dt_0$ were chosen. As figure 5 shows, velocity profile with $0.1 \times dt_0$ and $10 \times dt_0$ are very close to velocity profile of the reference time step case. However, for time step of $100 \times dt_0$ the velocity profile becomes incorrect.

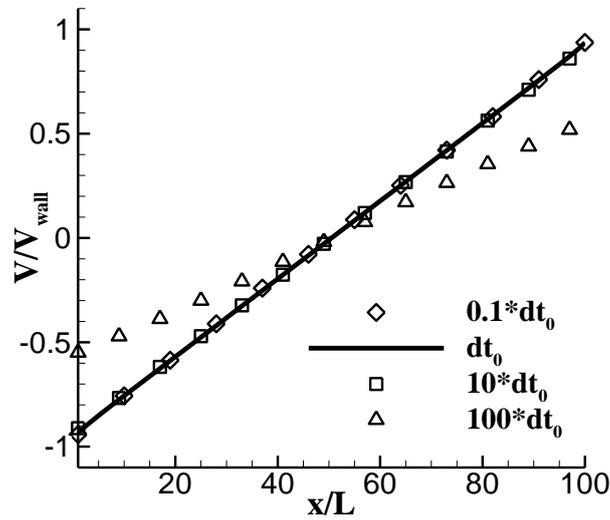


Figure 5: Time step comparison ($dt_0 = 2 \times 10^{-8}$)

2.3.5. Knudsen comparison

As seen in figure 6, Fokker-Planck works very accurately at low Knudsen numbers. This can be very useful in hybrid DSMC Fokker-Planck method which for low Knudsen numbers Fokker-Planck and for higher Knudsen numbers DSMC can be implemented. Figure 6 Shows that Fokker-Planck can be very accurate for a variety of Knudsen numbers.

As seen in figure 6 (d) for $KN=0.3$ there is a little difference in velocity profile near walls which backs to variations in Knudsen layer.

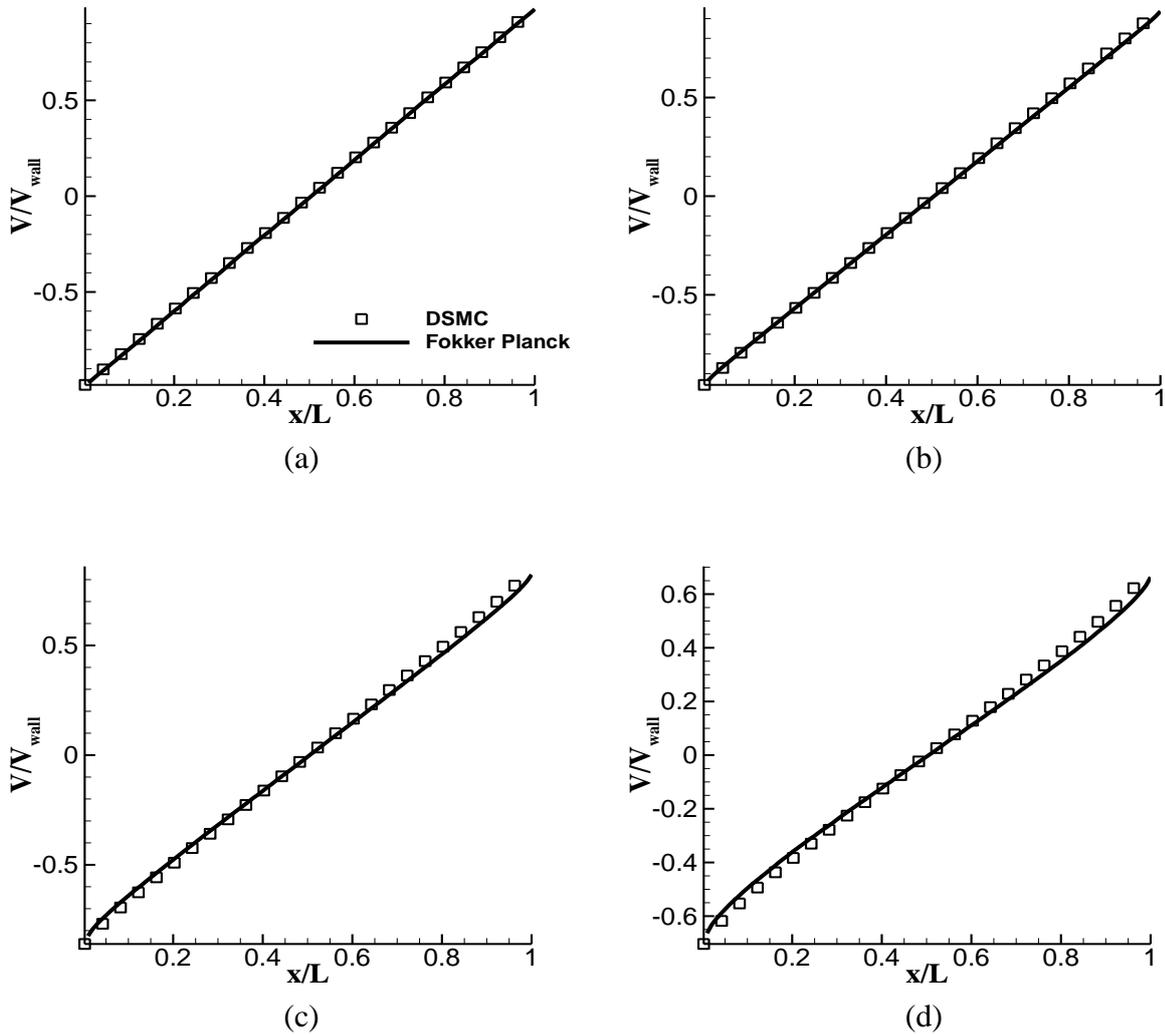


Figure 6: Knudsen comparison of couette flow a) $KN=0.005$ b) $KN=0.0237$ c) $KN=0.1$ d) $KN=0.3$

2.3.6. Fourier heat conduction

The other problem which was chosen for verification is Fourier heat conduction. This problem considers two parallel walls with two different temperatures and no movement for any of the walls. Assuming infinitely long walls, the temperature became one dimensional. Figure 7 shows the schematic diagram of Fourier heat conduction.

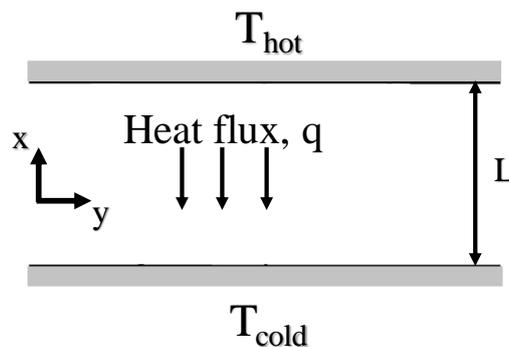


Figure 7: A schematic diagram of Fourier heat conduction

We considered heat conduction of Maxwellian Argon gas for two cases, which will be mentioned below.

2.3.7. Verification

Fourier heat conduction is a very sensitive case. Therefore, two cases for verification was chosen. For a good comparison, analytical results and DSMC-SBT results from a newly published paper were considered.¹³

For case 1, Argon gas at $Kn = 0.001$, $T_{cold} = 173.15$ K, $T_{hot} = 373.15$ K was examined. The result is presented in Figure 8(a) and for case 2, $Kn = 0.024$, $T_{cold} = 223.15$ K, $T_{hot} = 323.15$ K was considered, and the result is presented in Figure 8(b).

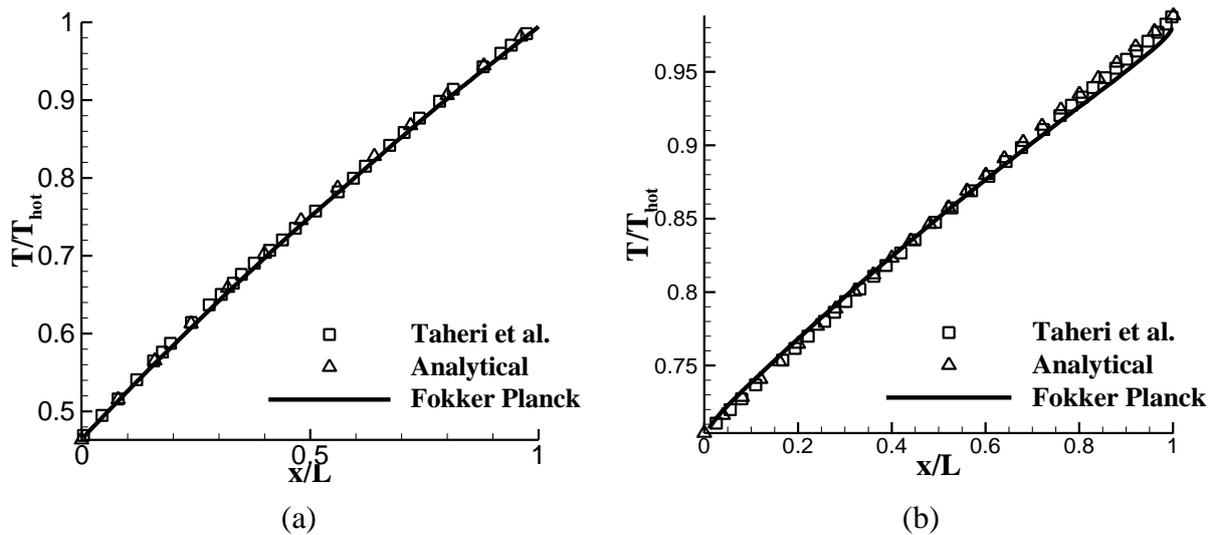


Figure 8: Comparison between DSMC-SBT (square)¹³, analytical solution (delta) and Fokker Planck (line) for Case 1 (a) and Case 2 (b)

As the results show, Fokker Planck solution captures DSMC-SBT and analytical data very well.

3. Conclusions

This paper shows the best grid and PPC for this simple cubic Fokker-Planck method. The Fokker-Planck method is accurate in a wide range of Knudsen number and results were validated with DSMC method. Time step change shows no such difference between Fokker-Planck and DSMC. This is a crucial issue because bigger time steps can converge the results much faster. Finally, the Fokker-Planck method could be integrated into the computational procedure of the DSMC method in order to reduce computational costs for applications with a broad range of Knudsen number.

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