A novel algorithm for implementing a specified wall heat flux in DSMC: Application to micro/nano flows and hypersonic flows

Hassan Akhlaghi\textsuperscript{a,b}, Ehsan Roohi\textsuperscript{a,∗}

\textsuperscript{a}Aviation Technology Research Institute, Ferdowsi University of Mashhad, P.O. Box: 91775-1111, Mashhad, Iran
\textsuperscript{b}High Performance Computing (HPC) Laboratory, Department of Mechanical Engineering, Faculty of Engineering, Ferdowsi University of Mashhad, P.O. Box: 91775-1111, Mashhad, Iran

\textbf{ARTICLE INFO}

Article history:
Received 4 July 2015
Revised 20 October 2015
Accepted 15 December 2015
Available online 29 December 2015

Keywords:
DSMC
Rarefaction
Specified wall heat flux
Controlling factor
Modified iterative technique (MIT)
Hybrid MIT–ITS

\textbf{A B S T R A C T}

This paper introduces a modified version of the iterative (IT) technique called the modified iterative (MIT) technique which implements a desired wall heat flux distribution over the wall for rarefied gas simulations using the direct simulation Monte Carlo (DSMC) method. The accuracy of the MIT technique and suitable ranges of employed parameters are examined in various test cases, namely, shear driven Couette and cavity flows, hypersonic/supersonic flows over flat plate/cylinder, and pressure/inertia-driven flows through micro/nanochannel. In each simulated test case, rarefied gas is considered in the presence of the wall with the specified heat flux distribution. We show that the controlling factor is a critical parameter that affects the speed of wall temperature update. This parameter should be selected appropriately for faster solution convergence. Additional considerations in the MIT technique are also presented and investigated. The possibility of employing an efficient hybrid approach based on MIT and inverse temperature sampling (ITS) techniques for implementing the specified wall heat flux is also examined.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

Rarefied gas dynamics is a diverse field, encompassing, for example, high altitude hypersonic flow fields, the reflective and reactive characteristics of gases interacting with solid and liquid surfaces, energy transfer phenomena in molecular collisions, aerosol dynamics, cluster formation and topology, flows induced by evaporation and condensation, upper-atmospheric dynamics, and the attainment of milli-Kelvin temperatures by flow cooling techniques [1]. In rarefied gas flows, the molecular mean free path ($\lambda$) is comparable with respect to the length scale of flow properties changes (L). In such flows, analysis must be performed using accurate approaches based on the solution of the Boltzmann equation [2].

In many of the above-mentioned flows, gas-surface heat transfer plays an essential role in flow field properties. For this reason, developing computational tools for simulation of rarefied gas flows under controlled gas-surface heat exchange is crucial for the study of flow physics and thermal engineering applications. There are several techniques for implementation of specified wall heat flux in rarefied gas flows using analytical, molecular, and continuum-based approaches [3–19]. In some rarefied gas simulations [20–22], adiabatic wall condition have been performed by employing equal temperatures for gas and surface, especially for low-speed flows. It is a simple way for simulation of adiabatic wall condition in low-speed flows. This adiabatic wall condition could be named as both uniform wall temperature (UWT) as well as uniform wall heat flux (UWH) conditions. There are numbers of publications, for example [3–5], which implement specified wall heat flux in analytical and continuum-based approaches using adjusting the temperature gradient near the wall:

$$q_w = -k \frac{\partial T}{\partial n} \bigg|_{n=0}, \quad (1)$$

where $k$ is the conductivity and $n$ is the direction normal to the wall. Using Eq. (1) and temperature jump condition, wall temperature is obtained. Temperature jump condition is used for slip flow modeling in analytical, and continuum-based analyzes of rarefied gas flow [5]:

$$T_w = T \bigg|_{n=0} - \left[ \frac{\alpha \lambda}{n} - \beta \lambda^2 \frac{\partial^2 T}{\partial n^2} \right]_{n=0}. \quad (2)$$

where $\lambda$ is the local mean free path and $\alpha$, $\beta$ correspond to first-order and second-order slip models, respectively. Temperature profile adjacent to the wall can be solved analytically or numerically. Then, wall temperature is obtained from the implemented wall heat flux.

Continuum-based approaches are valid for slip and early transitional flow regimes [23,24]. At highly rarefied conditions,
molecular methods are employed for a description of flow fields instead of continuum-based ones. In molecular dynamic (MD) simulations [6–11], the heat flux in a periodic region could be created by exchanging velocities of the particles in "cold" and "hot" slabs located in the middle of the simulation box and adjacent to one of the simulation box boundaries. This exchange periodically results in the heating up of the hot slab and cooling down of the cold slab and finally leads to a steady-state temperature gradient due to thermal conduction through slabs [7]. The imposed heat flux is as:

\[
\langle J(t) \rangle = \sum_{\text{transfers}} \frac{m}{2} (v_c^2 - v_h^2).
\]

(3)

where \(v_c\) and \(v_h\) are the velocities of particles correspond to cold and hot slabs. The new and old velocities after and before the exchange are related according to [8]:

\[
\begin{align*}
    v_{\text{new}}^c &= v_{\text{old}}^h \\
    v_{\text{new}}^h &= v_{\text{old}}^c
\end{align*}
\]

(4)

There are several published papers that present numerical techniques for implementation of wall heat flux in the direct simulation Monte Carlo (DSMC) method [12–17,19]. Genovesi [12] implemented an adiabatic viscous wall by taking the magnitude of the particle speed as a constant through a collision with the wall. A uniform distribution was assigned for the direction of reflected particles. Wang et al. [13–15] introduced an inverse temperature sampling (ITS) technique to implement specified wall heat flux (SWH) boundary condition in the DSMC method. In the ITS technique, the local wall temperature is obtained from the local specified gas-surface heat exchange (\(\Delta \epsilon\)) as:

\[
T_w = \frac{\epsilon_{\text{inc}} - \Delta \epsilon}{\kappa (4 + \zeta_{\text{rot}})/2},
\]

(5)

where \(\kappa\) and \(\zeta_{\text{rot}}\) correspond to the incident energy flux, Boltzmann constant, and number of rotational degrees of freedom, respectively. Their results showed that the ITS technique would be able to impose the specified heat flux rate distribution correctly at the wall. ITS technique also was modified for multi-atomic gasses [15]. Inappropriate initial wall temperature distribution or severe cooling condition may lead to negative unphysical wall temperature values during the simulation [17]. Tzeng et al. [18] presented a wall-fluid molecule collision rule for the description of an adiabatic solid-wall boundary condition in atomistic simulations of rarified gas natural convection. In this method, the magnitude of the particle velocity is kept invariant before and after the collision. The normal velocity component is reversed with the same magnitude.
while the other two components can vary randomly [16]. Akhlaghi et al. [17] previously introduced an iterative (IT) technique for implementation of desired wall heat flux distribution in DSMC simulations. In the IT method, local wall temperature is corrected during the simulation according to the comparison of obtained wall heat flux ($q_w$) with the desired or expected wall heat flux ($q_{d_{es}}$) as follows [17]:

$$T_{new}^w = T_{old}^w \left(1 + RF \frac{q_w - q_{d_{es}}}{|q_{d_{es}}| + \varepsilon_0} \right)$$

(6)

RF is a relaxation factor to control the convergence. Adjusting an efficient value for RF depends on the various parameters such as implemented wall heat flux magnitude, flow rarefaction, wall properties sampling period ($\Delta t$), and number of particles impinging on the wall. There is also another consideration in the selection of $\varepsilon_0$ which is a positive non-zero energy flux and should be negligible in comparison with the incident energy fluxes. It is defined for preventing zero denominator condition in an adiabatic wall case.

In the current paper, we present a modified iterative (MIT) technique. MIT technique is based on the normalized heat flux parameter, and it is free from some complexities of the IT technique. In this technique, wall temperature is modified during the DSMC simulation based on the deviation of the normalized heat flux from the desired one. Contrary to the IT, MIT technique does not require additional consideration for the adiabatic wall case. The capability of the MIT technique is measured for a broad range of benchmark test cases of rarefied gas flow, i.e., shear-driven Couette and cavity flows, hypersonic-supersonic flows over flat plate/cylinder, and pressure-/inertia-driven flows through micro/nanochannel. The effects of various main parameters of the MIT technique are examined, and the suitable ranges of these parameters for each test case are proposed. Some improvements in the MIT technique are also investigated. Here we also describe an efficient MIT- and ITS-based hybrid method capable of achieving smooth variations of wall temperature, i.e., minimum fluctuations, while preserving acceptable convergence speed. One important potential application of the proposed technique is its use with a radiative equilibrium wall boundary condition, where the convective heat transfer to the surface is balanced by the thermal radiative emission which is a very important boundary condition for hypersonic flow modeling.

2. Numerical method

2.1. DSMC method

DSMC is one of the most successful particle simulation methods in treating rarefied gas flows. It is a numerical tool to solve the Boltzmann equation based on the direct statistical simulation of the molecular processes described by the kinetic theory [25]. DSMC uses a finite set of model particles that move and collide in a computational domain to perform a stochastic simulation of the real molecular gas dynamic behavior. The basic concept of the method is built on a discretization in time and space of the real gas dynamics process and splitting the motion into two successive stages of free molecular motion and binary intermolecular collisions within the grid cells in each time step [26]. In the DSMC implementations used in this work, the generalized hard sphere (GHS) collision model [27] is utilized to consider the accurate variation of the viscosity with the temperature over a broad range of temperature variations. This model is an extension of the variable hard sphere (VHS) model to include terms that allow modeling of molecules with both repulsive and attractive potentials. The choice of the collision pair is done based on the no time counter (NTC) method [25]. Here, monatomic argon, $m = 6.63 \times 10^{-26}$ kg and $d = 4.17 \times 10^{-10}$ m, is considered as the working fluid. The simulation results have been performed by using various DSMC solvers developed by Akhlaghi and co-workers [17,22,28–32].
Fig. 5. Effect of $\alpha$ in the convergence of the MIT technique in the case of Couette flow at various degrees of flow rarefaction, $Kn = 0.01, 0.1, \text{ and } 1.0$. 
Fig. 6. Effect of $\Delta t_{WS}$ in the convergence of the MIT technique in the case of Couette flow at various degrees of flow rarefaction, $Kn = 0.01$, 0.1, and 1.0.
2.2. Molecular gas-surface interaction

There is a gas-surface energy exchange when a particle collides with a surface. The thermal accommodation coefficient ($\alpha_c$) represents the fraction of energy transferred between the surface and the particle as follows [25]:

$$\alpha_c = \frac{E^{inc} - E^{ref}}{E^{inc} - E^w}$$  \hspace{1cm} (7)

Superscripts “inc” and “ref” refer to the incident and reflected energy fluxes. $E^w$ is the reflected energy flux if the molecular reflective characteristic temperature is equal to the wall temperature. There is a complete thermal accommodation for the diffusive wall, i.e., $\alpha_c = 1$. In the case of specular wall ($\alpha_c = 0$), the energy transferred between surfaces and molecule is zero. Hence, the specular wall can be referred as “inviscid adiabatic wall”. The walls in the current paper are treated as diffusive in which the velocity of reflected molecules is randomly attributed according to one-half-range Maxwellian distribution that is determined via the wall.
temperature magnitude as follows [25]:

\[
\begin{align*}
    u_{ref} &= \sqrt{-\log(R_f)V_{mp} \sin(2\pi R_f)} \\
    v_{ref} &= \sqrt{-\log(R_f)V_{mp}} \\
    w_{ref} &= \sqrt{-\log(R_f)V_{mp} \cos(2\pi R_f)},
\end{align*}
\]

(8)

where \(V_{mp} = \sqrt{2RT}\) is the most probable thermal speed of the particles at the wall temperature and \(R\) is the gas constant. \(R_f\) is a uniformly distributed random number between 0 and 1.

The wall heat flux rate is determined by sampling over the impinging particles to the wall cell:

\[
    q_w(x) = \left(\sum_{i=1}^{N_{CM}} \epsilon_{tr} + \sum_{i=1}^{N_{CM}} \epsilon_{rot} + \sum_{i=1}^{N_{CM}} \epsilon_{vib}\right)_{inc} - \left(\sum_{i=1}^{N_{CM}} \epsilon_{tr} + \sum_{i=1}^{N_{CM}} \epsilon_{rot} + \sum_{i=1}^{N_{CM}} \epsilon_{vib}\right)_{ref} / \Delta t_{WS} S N_0,
\]

(9)

where \(N_{CM}\) and \(N_0\) are the number of impinging particles to the wall surface and the number of real molecules represented by one simulated particle, respectively. \(\Delta t_{WS}\) is the time interval of wall properties sampling and \(S\) is the wall surface area. The values of \(\epsilon_{tr}\), \(\epsilon_{rot}\), and \(\epsilon_{vib}\) are translational, rotational, and vibrational energies of impinging particles.

2.3. Modified iterative technique (MIT)

In the previously proposed IT technique [17], the local wall temperature is corrected during the simulation for imposing a desired wall heat flux \(q_{des}\) distribution according to the following formula:

\[
    \Delta T_w = T_{wRF} \frac{q_w - q_{des}}{|q_{des}| + \epsilon_0}
\]

(10)

Where \(q_w\) and \(q_{des}\) are desired and obtained local wall heat flux rates. The final results will be obtained from sampling after reaching converged wall temperature distribution. Adjusting the relaxation factor \(RF\) in a manner that ensures the convergence behavior depends on the desired wall heat flux magnitude, flow rarefaction, wall properties sampling period, and number of DSMC particles impinging the wall. The value of 0.03 has been recommended for RF in [17]. However, it is complex to determine an efficient value for RF in each case. On the other hand, \(\epsilon_0\) which is defined for the adiabatic wall, is a positive non-zero value that should be considered small compared to the incident energy flux. Choosing a
low RF value leads to very slow convergence. Also, larger values of RF result in the solution divergence due to significant fluctuations of $q_w$.

In the current paper, we introduce the MIT technique that improves the difficulties mentioned above. In the MIT, wall temperature correction is obtained based on the normalized wall heat flux values as follows:

$$\Delta T_w = \alpha (q_w^* - q_{des}^*) T_w,$$

(11)
Fig. 13. Effect of $\alpha$ in the convergence of the MIT technique in the case of the cavity flow at various degrees of flow rarefaction, i.e., $Kn = 0.01, 0.1,$ and $1.0$. 
where $\alpha$ is a factor in controlling the convergence. Contrary to the IT technique, it is not required to use $\varepsilon_0$ in the adiabatic wall case. Like the IT technique, MIT is also based on a simple physical concept: lower magnitude of the negative (heating) wall heat flux should result in an increase in the wall temperature and higher heating wall should result in decreasing in the wall temperature. The normalized local wall heat flux parameter ($q^*_w$) is defined as the ratio of the gas-surface energy transfer rate to the flow energy rate \cite{17,31}:

$$q^*_w = \frac{q_w}{q_f} \quad (12)$$

The denominator is a characteristic energy flux rate calculated based on the macroscopic flow properties as follows:

$$q_f = C_p \rho_o U_o T_o, \quad (13)$$

where $C_p$ is the specific heat of gas and $\rho_o$, $U_o$, and $T_o$ are reference values for density, velocity, and temperature, which are properties of the simulation. According to Eqs. (12 and 13), wall heat value is normalized by flow reference values. Therefore, it is possible to determine an optimum range of $\alpha$ applicable to various cases of rarefied gas flow simulations. Eqs. (11–13) also counts the effect of flow rarefaction by considering the flow density in the normalization process.

Eq. (11) corrects wall temperature during the DSMC simulation to achieve a desired wall heat flux. Before the convergence of flow and wall properties, the sampling is performed at the specified time intervals for flow ($\Delta t_{FS}$) and wall ($\Delta t_{WS}$). Each interval time consists of large numbers of DSMC time steps ($\delta t_{DSMC}$). At the end of each time interval, convergence criteria are checked, and samplings of flow/wall properties are initiated. Just before the final convergence, different sampling time values are used for the wall and flow properties. After reaching convergence, sampling over the wall and flow properties is performed over a wide time interval. Different values for $\Delta t_{FS}$ and $\Delta t_{WS}$ are selected because that allows easy controlling of the MIT technique. $\Delta t_{WS}$ is selected based on the robustness, accuracy, and convergence speed of the MIT technique. The flow properties sampled before convergence are used to track flow characteristics during simulation, determine cell temperature for intermolecular collision handling, and implement boundary conditions during simulation.

It is aimed to avoid error accumulation due to delays in implementation of Eq. (11). This equation is applied at the end of each $\Delta t_{WS}$ (Fig. 1). After surface properties converge, especially wall temperature, sampling is started for a long time to reduce statistical fluctuations.

### 3. Comparison of ITS, IT, and MITs

The MIT technique, Eq. (11), is actually an improved version of the IT technique, i.e., Eq. (10). The MIT technique is based on the normalized values of wall heat flux; as it is simpler to determine the normalized values of wall heat flux for the wall boundary condition than using dimensional values, which vary with flow rarefaction. In the case of small wall heat flux values, determination of RF requires some additional considerations to ensure the stability of the IT technique; MIT, however, needs a suitable definition for a reference wall heat flux value, for which we present different benchmark test cases in this paper. Detailed discussions on the differences between the IT and ITS techniques were previously reported in \cite{17}.

In this section, a convergence study is conducted between ITS, IT, and MIT techniques. For this, we have considered Couette flow with a constant temperature (500 K) moving wall and adiabatic stationary wall (See Fig. 4). Adiabatic wall condition is imposed...
using three different approaches, i.e. ITS, IT, and MIT techniques. The simulation results are obtained for Kn = 0.1 and Mach number based on the lid velocity equal to 0.2. Fig. 2 shows the convergence speed by considering the variations of wall temperature and normalized heat flux distributions for ITS and MIT techniques at various values of $\alpha$. The trends are plotted using least-squared lines with specified scatterings. As it is seen, the convergence rate for lower values of $\alpha$ is slower but the fluctuations in wall temperature and the corresponding heat flux are less. The simulation results indicate that the desired zero wall heat flux have been obtained by both MIT and ITS techniques. Wall temperature fluctuations for $\alpha = 2$ and ITS cases are significant compared with those of $\alpha = 0.1$ and 0.5.

Fig. 3 compares the convergence rate for both ITS and IT methods for various values of RF. Convergence for lower values of RF is slower, but fluctuations in wall temperature variations are less. Zero wall heat flux has been obtained by both techniques. Our investigations showed that the IT technique fails and wall temperature diverges for RF = 0.1. Fluctuations in wall temperature for ITS and IT techniques with RF = 0.03 are more. It should be mentioned that fluctuations in the wall temperature and heat flux will be diminished with sampling over a large interval time; however, here we show and compare solutions of all techniques during a specified period.

4. Results and discussions

4.1. Benchmark test cases

In the current section, the capability of the MIT technique is evaluated for various benchmark test cases of rarefied gas flow. The selected test cases are famous problems in rarefied gas flow investigations [33–36]. We consider micro/nano-Couette flow, supersonic flow over a flat plate, Poiseuille flow (or pressure-driven flow) through micro/nanochannel, supersonic flow (or inertia-driven flow) through microchannel, micro/nano-cavity flow, and hypersonic flow over a cylinder subject to the walls with specified heat flux rate (SWH). Implementation of Eq. (11) needs to determine the reference values for density, temperature and velocity. Table 1 lists the reference values for various simulation cases.

4.2. Couette flow

Fig. 4 shows the geometry and imposed boundary conditions for rarefied Couette flow under specified wall heat flux condition. Black line indicates the moving wall with desired wall temperature (UWT) and gray line corresponds to a stationary wall with uniform wall heat flux (UWH) distribution. The walls are separated
Fig. 18. Effect of $\Delta t_{WS}/\delta t_{DSMC}$ on convergence of wall heat flux distribution; $Kn = 0.1$ and $\alpha = 0.2$.

Fig. 19. Effect of $\alpha$ on convergence of wall heat flux distribution; $Kn = 0.01$.

by a distance of $H$. Desired wall temperature and heat flux values for moving and stationary walls are denoted by $T_{avg}$ and $q_{avg}$, respectively. Knudsen number is defined as $Kn = \lambda_{avg}/H$, where “avg” refers to an averaged value.

The moving wall with a temperature of 300 K and a distance of 1.0 μm is considered. The Mach number based on the upper wall velocity is equal to 0.2. Fig. 5 shows the effect of controlling parameter ($\alpha$) on the convergence of the MIT technique for various Knudsen numbers of 0.01, 0.1, and 1.0. The value of $q_{w}^{*} = -0.5$ is set to the bottom wall that heats the flow. The ratio of $\Delta t_{WS}$ to $\delta t_{DSMC}$ is set to $4 \times 10^5$ for various cases. The horizontal axis corresponds to the normalized simulation time, i.e., number of DSMC time step. As it seen, higher $\alpha$ increases the convergence speed and fluctuations in the resultant wall temperature distributions. A
Effect of $\alpha$ in the convergence of the MIT technique in the case of flat plate flow at $\text{Kn}_{0.1}$.

Fig. 21. Wall heat flux and corresponding wall temperature distributions under cooling, adiabatic, and heating wall conditions in the case of flat plate flow at $\text{Kn} = 0.01$.

large $\alpha$ leads to a divergence in the MIT solution. At lower Knudsen numbers, $\alpha$ could be chosen larger, see $\text{Kn} = 0.01$ case.

Effect of wall sampling interval time ($\Delta t_{WS}$) on the convergence of the MIT is investigated in Fig. 6. The results are presented for various levels of flow rarefaction. The magnitude of $\alpha$ is set to 0.5 for different cases. It is well seen that convergence is slower for higher values of $\Delta t_{WS}$, but the obtained wall heat flux and temperature are smoother.

Fig. 7 compares the normalized velocity profiles obtained by the MIT technique for adiabatic bottom wall ($q^*_w = 0.0$) with the first and second order analytical solutions [24] for the isothermal Couette flow. The figure indicates that the results of MIT
technique have a suitable agreement with those of analytical solutions.

Fig. 8 shows the normalized heat flow ($q^*$) through the domain. Normalized heat flow is defined similar to Eq. (12) using normal heat flow component in the simulation domain. Heat flow vector is defined as follows [25]:

$$ q = \frac{1}{2} \rho c' c' + n e_{rot} c' $$

(14)

where $n$ and $c'$ are number density and peculiar velocity vector, respectively. Fig. 6 illustrates the $q^*$ distributions from the stationary bottom wall ($Y = 0.0$) to upper moving ($Y = 1.0$) one. The results are presented for $Kn = 0.01$, 0.1, and 1.0 under different bottom wall conditions, i.e., heating ($q^*_w = -0.1$), cooling ($q^*_w = 0.1$), and adiabatic ($q^*_w = 0.0$).

According to Fig. 8, $q^*$ distribution is approximately uniform and equal to $q^*_w$ for $Kn = 0.01$ (circles). At higher rarefied conditions of $Kn = 0.1$ (triangles) and $Kn = 1.0$ (squares), $q^*$ continuously increases from the bottom wall to the upper one due to viscous heating effects. Comparing triangles and squares indicates that this increase is higher for more rarefied conditions. Similar to temperature jump condition and velocity slip concepts [24], there is also a jump condition between $q^*_{Y=0}$ and $q^*_w$ which increases with $Kn$.

In $Kn = 0.01$ condition, the magnitude of $q^*_w = 0.1$ leads to an unphysical negative wall temperature. In the case of near-continuum flow, the magnitude of cooling wall heat flux is larger for the same $q^*_w$ because of a higher density; see Eq. (13). The negative wall temperature value means that the desired heat flux being removed from the wall is greater than the incoming energy flux level. Based on the MIT technique, wall temperature is reduced to reach the desired level of cooling. When the desired heat flux removed from the wall is greater than the incoming energy flux level, it leads to unphysical negative wall temperature.

Fig. 23. Effect of $\alpha$ in the convergence of the MIT technique in the case of supersonic flow through micro/nanochannel at Kn = 0.01.
Fig. 9 shows the geometry and imposed boundary conditions for the rarefied gas flow in a square Cavity. Black line indicates the moving lid wall with UWT condition and gray lines correspond to stationary surrounding walls under UWH condition. The cavity length scale is considered as \( L = 1.0 \mu m \). Moving lid wall has a uniform temperature distribution of 500 K and the Mach number equal to 0.2 based on \( T_{\text{des}} \). Knudsen number is defined as \( Kn = \frac{\lambda_{\text{init}}}{L} \). Subscript “init” refer to the initial density in the domain.

Figure 10 shows the convergence behavior of the average intermolecular collision rate (ICR) versus the normalized simulation time. The flow Knudsen number is 0.1 and the normalized wall heat flux for surrounding walls is equal to \(-0.1\), which denotes the heating condition. The dashed line corresponds to convergence limit, after which sampling of properties could be performed.

Figs. 11 and 12 show the convergence behavior of the MIT in the form of normalized wall heat flux (Fig. 11) and obtained wall temperature (Fig. 12) distributions. As it seen, at the initial step, surrounding walls have a uniform temperature distribution equal to moving lid wall, i.e., \( T_{\text{des}} \), which leads to an initial wall heat flux distribution approximately equal to zero (solid line). After that, wall heat flux approaches to the desired uniform distribution equal to \( q^*_w = -0.1 \) with modification of the temperature of wall cells during the simulation.

According to the results, at simulation time \( t/\delta t_{\text{DSMC}} = 1.2 \times 10^5 \) convergence in wall temperature distribution has been reached. There are fluctuations in the heat flux and temperature distributions that are eliminated by taking higher \( \Delta t_{\text{WS}} \) values or continuing the simulation time. Moving lid wall has approximately an average wall heat flux equal to the sum of surrounding walls with opposite sign, i.e., 0.3. This means that heat entering the flow from the surrounding walls exits from the moving lid wall.

Fig. 12 investigates the effect of \( \Delta t_{\text{WS}} \) on the convergence behavior of the MIT technique for various flow rarefactions of \( Kn = 0.01, 0.1, \) and 1.0. The value of \( \alpha \) is set to 0.5 for different cases of \( \Delta t_{\text{WS}} \). Wall temperature and heat flux distributions for all cases are plotted at a particular simulation time of \( t/\delta t_{\text{DSMC}} = 8.0 \times 10^4 \). Lower values of \( \Delta t_{\text{WS}} \) lead to significant fluctuations and higher convergence speed. As it is seen, the required wall temperature for reaching \( q^*_w = -0.1 \) is higher for more dense flows. Comparing \( q^*_w \) distributions shows that the convergence is faster for more rarefied flows.

Fig. 13 demonstrates the effect of \( \alpha \) on the convergence of the MIT technique for different levels of flow rarefaction at a
Fig. 25. Comparison of wall properties for supersonic flows through microchannel under UWT (□) and UWH (◦) conditions at $Kn_{\infty} = 0.01; \alpha = 3$.

Fig. 26. Flow patterns, Mach contours, and isobaric lines for supersonic flows through microchannel under (a) UWT and (b) UWH conditions at $Kn_{\infty} = 0.01$.

Simulation time equal to $t/\delta_{\text{DSMC}} = 8.0 \times 10^4$. Higher $\alpha$ leads to faster convergence and more fluctuation. Fig. 14 presents the converged results for rarefied flow under heating (solid lines), cooling (dashed-dotted lines) and adiabatic (dashed lines) walls. It is well seen that surrounding walls (A-B, A-C, and B-D) have equal heat flux distributions. Moving lid wall has a uniform temperature and its heat flux magnitude is approximately equal to the sum of those of surrounding walls.

4.4. Hypersonic flow over a flat plate

Fig. 15 shows the geometry and imposed boundary conditions for the hypersonic rarefied gas flow over a flat plate. Black line indicates the specular reflector employed for more realistic inflow simulation [28,37,38]. Gray lines correspond to a flat plate with the length of $L$ under UWH condition. Hypersonic flow with specified free stream Mach number ($M_{\infty}$), temperature ($T_{\infty}$), and density ($\rho_{\infty}$) is considered. Knudsen number is calculated based on
Fig. 28. Effect of $\alpha$ on the convergence of MIT technique in the case of Poiseuille flow through microchannel at $Kn = 0.01$.

on the free stream properties and plate’s length, i.e., $Kn = \frac{\lambda_{\infty}}{L}$. For this study, hypersonic flow reported in Ref. [39] is considered where $M_{\infty} = 20.2$ and $T_{\infty} = 13.32$ K. A uniform cooling heat flux of $q_{w}^* = 2.0$ is considered for the plate.

Fig. 16 shows the convergence history of hypersonic flow under UWH condition using the MIT technique for two cases of $Kn = 0.01$ and 0.1. The results are presented for various values of $\Delta t_{WS}$ while the capturing parameter is the total heat transfer from the wall per unit depth of the plate. As it is seen, the convergence is faster for lower $\Delta t_{WS}$. The initial pick in the heat transfer values is related to the UWT DSMC simulations in the first wall sampling period of the simulation.
Effect of $\Delta t_{WS}$ on the wall heat flux distributions is also considered in Figs. 17 and 18. These figures plot wall heat flux distributions resulting from the MIT technique during UWH DSMC simulation. There are faster convergence and more fluctuations for lower $\Delta t_{WS}$.

Figs. 19 and 20 investigate the effect of $\alpha$ in the convergence of the MIT technique. As is expected, higher $\alpha$ leads to faster convergence. However, large $\alpha$ may result in divergence of the method, see case with $\alpha = 0.5$. 

Fig. 29. Effect of $\alpha$ on the convergence of MIT technique in the case of Poiseuille flow through microchannel at Kn = 1.0.
Fig. 21 shows the wall temperature and heat flux distributions obtained from the MIT technique for hypersonic flow over flat plate under UWH condition at \( Kn = 0.01 \). Taking enough simulation time leads to smooth results. Wall temperature distributions for cooling and heating walls are ascending and descending, respectively. The current results show that MIT technique enables implementing a desired wall heat flux distribution for the case of rarefied high-speed flows over a flat plate.

4.5. Inertia-driven flow through micro/nanochannel

Fig. 22 shows the geometry and imposed boundary conditions for the supersonic rarefied gas flow through a micro/nanochannel. The black line indicates the specular reflection region. Gray lines correspond to a micro/nanochannel with a length of \( L \) and height of \( H \) under UWH condition. The employed flow driven mechanism is an inertia force of supersonic inflow. Knudsen number is calculated based on the inflow condition and channel height, i.e., \( Kn = \frac{\lambda_{\infty}}{H} \). For this study channel \( M_{\infty} = 4.0 \) and \( T_{\infty} = 200 \) K is considered.

Supersonic inflow is choked at the conditions with uniformly heating or adiabatic walls. In these circumstances, there is a normal shock at the entrance, which turns supersonic flow to subsonic one. To maintain a supersonic inflow, we should select a suitable cooling wall heat flux. For this, we employ \( q_{w}^* = 0.07 \) and 0.4 for cases with \( Kn = 0.01 \) and 0.1, respectively. The \( q_{w}^* \) magnitudes less than mentioned values may lead to choking condition [28] and others large values may lead to unphysical negative wall temperature.

Now, the effect of \( \alpha \) on the convergence of the MIT is examined by capturing wall temperature and heat flux distributions during the simulation. The results have been shown for \( Kn = 0.01 \) and 0.1 in Figs. 23 and 24, respectively. The graphs indicate that the required time for achieving desired wall heat flux distribution is lower at higher \( \alpha \). The wall temperature at the beginning sections of the channel is significantly high. It is because of the presence of a shock at the entrance. This shock is weaker for more rarefied flow. For this reason, the wall temperature at the beginning sections is lower at \( \alpha = 0.1 \).

Fig. 25 compares wall properties, i.e., temperature, heat flux, collision rate, and pressure in both UWT and UWH conditions. Also, Fig. 26 compares flow patterns, Mach contours, and isobaric lines for two different conditions. The results are reported for the slip flow (\( Kn = 0.01 \)). For UWT case, wall temperature is equal to the inflow temperature that leads to a higher cooling wall heat flux at the initial sections compared to the UWH case. Higher cooling in the shock region leads to lower wall temperature distributions, less pressure on the wall (Fig. 25), weaker shock, and an extended high-velocity region (Fig. 26).

4.6. Poiseuille flow through micro/nanochannel

Fig. 27 shows the geometry and imposed boundary conditions for the pressure-driven or Poiseuille flow through a micro/nanochannel. Gray lines correspond to channel walls with the length of \( L \) and height of \( H \) under desired wall heat flux condition. The inflow temperature is equal to 500 K with inlet/outlet pressure ratio of 2. The channel has a length/height ratio of 10. Inflow pressure is different for any Knudsen number. For the evaluation of the MIT technique, the value of \( q_{w}^* = -0.02 \) is selected at all levels of flow rarefaction that corresponds to heating the flow by walls.

Figs. 28 and 29 investigate the effect of \( \alpha \) on the convergence of the MIT technique in the case of Poiseuille flow. As it is expected, high values of \( \alpha \) lead to faster convergence and a very higher value may result in divergence (\( \alpha = 3.0 \)). Investigations on the Poiseuille flows under specified wall heat flux have been reported in [17,22,29–31].

Figs. 30 and 31 compare wall temperature and heat flux distributions for Poiseuille flows under UWT and UWH conditions. The results of UWH cases are converged values obtained with \( \alpha = 1 \). It is seen that the averaged values of the wall heat flux is approximately zero for the Poiseuille flow under uniform wall temperature equal to the inflow temperature.

4.7. Supersonic flow over a cylinder

Supersonic/Hypersonic flow over the cylinder is an interesting simulation test case in rarefied gas flow studies [40,41]. We simulate rarefied supersonic/hypersonic flow over a cylinder to illustrate the capability of the MIT in the simulation of external aerodynamics. Consider a cylinder under UWH condition and with a diameter of \( D \), as shown in Fig. 32. A supersonic/hypersonic rarefied gas flow with Mach number of \( M_{\infty} = 5.0 \) and temperature of \( T_{\infty} = 200 \) K crosses over the cylinder. Knudsen number based on the cylinder diameter is equal to \( Kn = \frac{\lambda_{\infty}}{D} \).

There exists a wake region behind the cylinder. Hence, the wall heat flux in the behind wall region is approximately zero, independent of the wall temperature. For this reason, we set desired
Fig. 31. Comparison of wall heat flux and temperature distributions for Poiseuille flow through micro/nanochannel under UWT (□) and UWH (○) conditions at Kn∞ = 1.0.

Fig. 32. Geometry and imposed boundary conditions for supersonic flow over the cylinder.

Fig. 33. Wall collision rate and heat flux distributions during the simulation in the case supersonic flow over the cylinder under specified wall heat flux distribution at Kn∞ = 0.01.
cooling heat fluxes of $q_w^* = 0.8$ for the front ($0 \leq \theta < 66$) and $q_w^* = 0.0$ for the back ($66 \leq \theta \leq 180$) sections of the cylinder, respectively. The simulation results are obtained by the RGS2D solver [32].

Fig. 33 shows the convergence behavior of the wall collision rate (WCR) and heat flux distributions using the MIT technique during the solution. The squares correspond to the initial wall temperature distribution that is uniform and equal to the free stream value. As it is seen, a desired, step-shape heat flux distribution has been well implemented on the cylinder surface using the MIT. Fig. 34 compares the domain flow properties, i.e., temperature, Mach, density, and pressure for hypersonic flow over the cylinder under UWT and UWH conditions. In the case of UWT, wall temperature is equal to that of the free stream. Imposed wall heat flux distribution in UWH case results in a weaker cooling condition in comparison with the UWT case. This could be well observed in the wall heat flux distributions plotted in Fig. 33 where flow cooling in the front section of wall is more severe for UWT case. The weaker cooling by the front wall leads to an increase in the temperature and pressure and a decrease in the velocity behind the strong shock. Therefore, high-temperature, low-velocity, high pressure, and high density regions in UWH case are more extended compared to the UWT case. Moreover, the shock is farther from the body in UWH case.

5. Additional considerations in the MIT technique

5.1. Combined MIT–ITS technique (MIT-I)

There are some considerations in the MIT to further optimize this technique. For investigation of effects of these improvements, we consider the cases of adiabatic Couette flow and hypersonic flow over flat plate under adiabatic and heating conditions, as described in Section 4. First, we apply the ITS formulation to identify
Fig. 35. Convergence of the algorithm for basic initialization (MIT) and initialization based on the ITS technique (MIT-I) in the case of adiabatic Couette flow at \( K_n^{\infty} = 0.1 \).

Fig. 36. Convergence of MIT and MIT-I techniques in the case of hypersonic flow over the adiabatic flat plate at \( K_n^{\infty} = 0.1 \).

Fig. 37. Comparison of the basic MIT and MIT-II techniques one in the case of adiabatic Couette flow at \( K_n^{\infty} = 0.1 \).

An improved initial temperature distribution for the MIT technique, i.e., Eq. (5),

\[
T_{w, \text{init}} = \frac{q_{\text{des}}}{\kappa (4 + \zeta_{\text{rot}})}/2 \tag{15}
\]

Using Eq. (15) during the first steps of wall properties sampling \( \langle \Delta t_{WS} \rangle \), wall temperature is calculated based on the average energy exchanged by one incident molecule \( \langle q_{\text{des}} \rangle \). This magnitude is obtained from Eq. (9) as:

\[
q_{\text{des}} = \frac{q_{\text{des}} \Delta t_{WS} S}{N_c M_0} \tag{16}
\]

Fig. 35 compares the effect of different initial wall temperatures on the convergence of the MIT technique. The magnitude of \( \alpha \) is equal to 0.1, which leads to a slow convergence, see Fig. 2. In the basic initialization, which is labeled as “MIT”, the initial wall temperature is set to be equal to the temperature of the upper wall. “MIT-I” uses an alternative initialization approach that is based on Eq. (15). We found that the desired zero wall heat flux and corresponding wall temperature were obtained faster using the MIT-I technique compared to using the MIT technique.

Fig. 36 shows the distributions of wall temperature during the implementation of adiabatic wall using MIT and MIT-I techniques.
in the case of hypersonic flow over the flat plate. The magnitude of $\alpha$ is equal to 0.1 for two cases. All computational parameters for two cases are the same. For the primary MIT technique, initial temperature distribution, shown by Squares in Fig. 36, is uniform but in the case of MIT-I technique initial temperature distribution is non-uniform, and it is obtained from the ITS technique or Eq. (15). The convergence is faster for the MIT-I technique. Therefore, initialization based on the Eq. (15) considerably improves the speed of convergence. This enables the use of small values of $\alpha$, and consequently smooth wall temperature variation by preserving an acceptable convergence rate.

5.2. Use of a reference temperature (MIT-II)

An alternative approach is to employ a reference temperature instead of the wall temperature in Eq. (11) as follows:

$$\Delta T_w = \alpha (q^*_w - q^*_\text{des}) T_o,$$

which may decrease the fluctuations in the wall temperature. This approach also allows determination of the optimum value of $\alpha$. Based on Eq. (11), the convergence for heating cases is faster and fluctuations are greater because of the higher $T_w$ values in heating cases. Therefore, different values of $\alpha$ should be considered for heating and cooling cases. However, using Eq. (17) leads to the same speed for heating and cooling cases. We named the MIT based on Eq. (17) as “MIT-II”. Fig 37 compares wall temperature variations while applying an adiabatic wall condition using the basic MIT and MIT-II techniques for $\alpha$ values of 0.5 (red lines) and 2 (black lines). Thick and thin lines correspond to MIT and MIT-II solutions, respectively. The results indicate that applying Eq. (17) instead of Eq. (11), has negligible effects on obtained wall temperature fluctuations and the convergence speed.

Fig. 38 compares basic MIT and MIT-II techniques in the case of hypersonic flow over a cooling plate with $q^*_w = 2.0$ and $Kn = 0.1$, which was previously considered in Section 4. The value of $\alpha$ is set to 0.2 for both cases. Comparing with Figs. 37 and 38, the effect of applying MIT-II technique is more for the case of the flat plate. As the figure shows, reduction of temperature fluctuations is quite visible if we use MIT-II method.

5.3. A modified ITS technique

Finally, the effect of employing a controlling factor ($\beta$) in the ITS method is also investigated.

$$T_w^{\text{new}} = T_w^{\text{old}} + \beta \Delta T_w$$

In this approach, new wall temperature is obtained using Eq. (5) at the end of each $\Delta t_{WS}$, See Fig. 1. Then, the new wall temperature at the start of next $\Delta t_{WS}$ is calculated through updating the old temperature through Eq. (18), where correction wall temperature term ($\Delta T_w$) is defined as follows:

$$\Delta T_w = \frac{\varepsilon \text{inc} - \Delta \varepsilon}{\kappa (4 + \zeta_{\text{rot}})/2} - T_w$$

The factor $\beta$ controls the contribution of Eq. (5) in updating of the wall temperature. For $\beta = 1$, Eqs. (18) and (19) lead to the
primary ITS technique. Fig. 39 shows the effect of $\beta$ in the convergence of ITS method in the case of the adiabatic Couette flow. Similar to the MIT technique, a higher $\beta$ leads to more severe fluctuations in the wall temperature, but its effect on the convergence speed is quite negligible.

6. Conclusions

Current work presented the capability, robustness, and application of the MIT technique for simulation of rarefied gas flows under desired wall heat flux boundary condition in the DSMC method. Various benchmark test cases of rarefied gas flows, i.e., Couette and cavity flows, hypersonic/supersonic flows over the flat plate/cylinder, and pressure/inertia-driven flows through micro/nanochannel were considered to evaluate the MIT. Employing normalized values of the wall heat flux in the MIT technique leads to an easier selection of the controlling factor and prevention from additional considerations for small wall heat flux boundary conditions in the IT technique. The effect of different parameters of the MIT technique such as normalized wall heat flux, controlling parameter, and wall properties sampling period were investigated for various benchmark cases. The results indicated that the MIT technique well implements a desired heat flux distribution over the wall for different geometries and a broad range of working conditions. The suitable ranges of controlling factor also reported for various benchmark cases. However, a lower controlling factor leads to smooth wall properties but slower convergence. Additional considerations in the MIT technique were also presented and investigated for decreasing fluctuations and improving the convergence speed. An efficient hybrid method based on the MIT and ITS techniques (called MIT-I) was introduced and examined which leads to smooth variations of the wall temperature and preserving an acceptable convergence speed. Therefore, employing of the hybrid MIT–ITS is recommended. The proposed technique with a radiative equilibrium wall boundary condition can be employed as a useful boundary condition for hypersonic flow modeling.

Acknowledgement

The authors would like to thank Prof. Stefan Stefanov from Institute of Mechanics, Bulgarian Academy of Science for very helpful suggestions in developing the MIT-II technique.

References
