

Numerical simulation of a binary gas flow inside a rotating cylinder[†]

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Abstract

A new approach to calculate the axially symmetric binary gas flow is proposed. Dalton's law for partial pressures contributed by each species of a binary gas mixture (argon and helium) is incorporated into numerical simulation of rarefied axially symmetric flow inside a rotating cylinder by using the time relaxed Monte-Carlo (TRMC) scheme and the direct simulation Monte-Carlo (DSMC) method. The results of flow simulations are compared with the analytical solution and results obtained by Bird [1]. The results of the flow simulations show better agreement than the results obtained by Bird [1] in comparison with the analytical solutions. However, the results of the flow simulations using the TRMC scheme show better agreement than those obtained using the DSMC method in comparison with the analytical solutions.

Keywords: Boltzmann equation; TRMC; DSMC; Rotating cylinder

1. Introduction

In gas flow problems where the length scale of the system is comparable to the mean free path of molecules in the gas flow the concept of the continuum is no more valid, Knudsen number greater than 0.1 [1]. In this case the simulation is done by using the direct simulation Monte-Carlo (DSMC) or the collisional Boltzmann equation (CBE) methods [2, 3]. In most cases the direct solution of the CBE is impracticable due to the huge number of molecules; however, the implementation of the DSMC is often more practicable. So far a class of Monte-Carlo method has been used to simulate the rarefied gas dynamic problems. The rarefied hypersonic flow is solved by using the DSMC method by Bird [1]. The comparison between the Navier-Stokes and the DSMC methods for the simulation of the circumnuclear coma was done by Crifo et al. [4]. The simulation of the rarefied gas flow through circular tube of finite length in the tran-

sitional regime at both low Knudsen number and high Knudsen number is done by using the DSMC method by Shinagawa et al. [5]. More recently, Bottoni [6] used the molecular approach based upon a Monte-Carlo simulation for sodium vapor flow of monoatomic molecules in liquid metal fast breeder reactor bundle. Simulation of flows like recirculation flow problems or near continuum flows is still expensive due to the particular nature of the DSMC method [7]. However, Pareschi et al. [8] proposed a modification to the DSMC method to circumvent this problem. Pareschi et al. [9] used the time-relaxed Monte-Carlo (TRMC) method with the Wild sum expansion [10] to approximate the non-negative function describing the time evolution of the distribution function of particles. However, the optimal choice of the coefficients in the Wild sum expansion for the distribution function of particles is left as an open problem. Pareschi et al. [11, 12] simulated numerically the Boltzmann equation for a two-dimensional gas dynamic flow around an obstacle using the TRMC method. Their simulation showed improvement over the DSMC method in terms of computational efficiency. Nourazar et al. [13] compared the simulation of the

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Navier-Stokes and the Boltzmann equations of the axially symmetric compressible flow past a flat-nosed cylinder at high velocity and low pressure with shock wave using the Monte-Carlo method. The results of the two simulations are compared in terms of different Knudsen numbers.

1.1 Purpose of the present work

In the simulation of rarefied gas dynamic problems, when the Knudsen number is small, collisions occur at a fast rate; therefore, a kinetic treatment (DSMC) of the problem is extremely expensive due to the required small time-step. Since the ratio of time scales between macroscopic and microscopic effects is large enough, reaching the stationary results of flow characteristics may almost be impossible.

On the other hand, the TRMC schemes allow the use of larger time-steps than those required in the DSMC method, therefore allowing one to achieve the stationary results of flow properties in a comparatively shorter computational time. To our knowledge, none of the researchers so far tried to incorporate the new idea of using the Dalton’s law for the simulation of axially symmetric binary gas flow implementing the TRMC scheme. In the present work we intend to simulate the flow properties of a binary gas mixture (argon and helium) inside a rotating cylinder using the TRMC scheme and the DSMC method. The results of the simulations using the two methods are compared with the analytical solutions and the results obtained by Bird, [1] for the same case study problem. In the simulation using the DSMC we follow exactly the same procedures described in Bird, [1], and in the simulation using the TRMC we follow exactly the same procedures described in Pareschi et al. [12]

1.2 Description of the case study problem

A cylinder rotates at a tangential velocity of 1000 meter/second, and the radius of the cylinder is 1 meter. The gas mixture inside the cylinder contains 50% argon and 50% helium, the initial temperature of the gas mixture inside the rotating cylinder is 200 Kelvin, and the initial pressure of the gas mixture inside the cylinder is 2.76 Pascal absolute. These data are the same as those depicted by Bird [1].

2. Mathematical formulations

2.1 The Boltzmann Equation

The Boltzmann equation for the temporal evolution of particles velocity distribution function for species p is written as [1]:

$$\frac{\partial}{\partial t}(n_p f_p) + \mathbf{V}_p \cdot \frac{\partial}{\partial \mathbf{r}}(n_p f_p) = \frac{1}{\varepsilon} \sum_{q=1}^s Q(n_p f_p, n_q f_q) \tag{1}$$

In Eq. (1), n is the number density of molecules of species, f is the probability distribution function of the molecules of species having velocity \mathbf{V} , f_1 is the probability distribution function of the molecules of species having velocity \mathbf{V}_1 , ε is Knudsen number which is equal to the ratio of λ , the mean free path between collisions, to the characteristic length L . The subscripts p and q represent the particular species.

The bilinear collisional operator $Q(n_p f_p, n_q f_q)$ that describes the binary collisions of the molecules is given by:

$$Q(n_p f_p, n_q f_q) = \sum_{q=1}^s \int_{-\infty}^{+\infty} \int_0^{4\pi} n_p n_q [f_p^* f_{1q}^* - f_p f_{1q}] \sigma(|\mathbf{V}_{rpq}|, \Omega) d\Omega d\mathbf{V}_{1q} \tag{2}$$

Where, \mathbf{V}_{rpq} is the relative velocity between the molecules of species p and species q and Ω is a vector of the unitary sphere. The kernel σ is a non negative function which is described as [12]:

$$\sigma(|\mathbf{V}_{rpq}|, \Omega) = b_\alpha(\theta) |\mathbf{V}_{rpq}|^\alpha \tag{3}$$

Where, θ is the scattering angle between \mathbf{V}_{rpq} and $|\mathbf{V}_{rpq}| \Omega$. The variable hard sphere (VHS) [1] model is often used in numerical simulation of rarefied gases, where, $b_\alpha(\theta) = \varepsilon C$ with C a positive constant and $\alpha = 1$. The value of C is equal to [1], $C = \sigma_{pq}$.

Substituting Eq. (3) into Eq. (2) one gets the following:

$$\frac{1}{\varepsilon} Q(n_p f_p, n_q f_q) = \sum_{q=1}^s \int_{-\infty}^{+\infty} \int_0^{4\pi} n_p n_q \sigma_{pq} V_{rpq} [f_p^* f_{1q}^* - f_p f_{1q}] d\Omega d\mathbf{V}_{1q} \tag{4}$$

Substituting the bilinear collisional operator (Eq. (4)) into Eq. (1), the Boltzmann equation is written as:

$$\begin{aligned} & \frac{\partial}{\partial t}(n_p f_p) + \mathbf{V}_p \cdot \frac{\partial}{\partial \mathbf{r}}(n_p f_p) \\ &= \frac{1}{\varepsilon} Q(n_p f_p, n_q f_q) \\ &= \sum_{q=1}^s \int_{-\infty}^{+\infty} \int_0^{4\pi} n_p n_q \sigma_{pq} V_{r,pq} [f_p^* f_q^* - f_p f_q] d\Omega dV_q \end{aligned} \tag{5}$$

In Eq. (5), n is the number density of molecules of species, f is the probability distribution function of the molecules of species having velocity \mathbf{V} , f_1 is the distribution function of the molecules of species having velocity \mathbf{V}_1 , f^* is the post-collision probability distribution function of the molecules of species having velocity \mathbf{V} and f_1^* is the post-collision probability distribution function of the molecules of species having velocity \mathbf{V}_1 . The subscripts p and q represent the particular species.

2.2 The TRMC Scheme

In a binary gas mixture flow with two different species p and q , the Boltzmann equation can be written for the species separately.

$$\begin{aligned} & \frac{\partial}{\partial t}(n_p f_p) + \mathbf{V}_p \cdot \frac{\partial}{\partial \mathbf{r}}(n_p f_p) \\ &= \frac{1}{\varepsilon} Q(n_p f_p, n_p f_p) + \frac{1}{\varepsilon} Q(n_p f_p, n_q f_q) \end{aligned} \tag{6}$$

In the present work the Dalton law is used to calculate the pressure; the pressure of the mixture is calculated as $P = P_p + P_q$, where P_p is the partial pressure of the species p , and P_q is the partial pressure of the species q . The density of the mixture is calculated as $\rho_m = y_{Ar} \rho_{Ar} + y_{He} \rho_{He}$, where ρ_m is the mixture density, y_{Ar} is the molar fraction of argon, ρ_{Ar} is the density of argon, y_{He} is the molar fraction of helium and ρ_{He} is the density of helium. First, we assume that only the argon gas exists inside the rotating cylinder and the flow is simulated by using the TRMC and the DSMC methods. Second, we assume that only the helium gas exists inside the rotating cylinder and the flow is simulated by using the TRMC and the DSMC methods. In both cases the effect of collisions of molecules of argon and the effect of collisions of molecules of helium are considered separately, $Q(n_p f_p, n_q f_q) = 0$.

$$\begin{aligned} & \frac{\partial}{\partial t}(n_p f_p) + \mathbf{V}_p \cdot \frac{\partial}{\partial \mathbf{r}}(n_p f_p) = \\ & \frac{1}{\varepsilon} Q(n_p f_p, n_p f_p) \end{aligned} \tag{7}$$

We split Eq. (7) [14] into an equation for the effect of collision, $\partial(n_p f_p) / \partial \mathbf{r} = 0$, and an equation for the effect of convection, $Q(n_p f_p, n_p f_p) = 0$. The equation for the effect of collision is written as [12]:

$$\frac{\partial}{\partial t}(n_p f_p) = \frac{1}{\varepsilon} Q(n_p f_p, n_p f_p) \tag{8}$$

For simplicity we omit the index and replace $n_p f_p$ with f , where f is the mass density function of the molecules of species having velocity \mathbf{V} . Then Eq. (8) is written as:

$$\frac{\partial}{\partial t}(f) = \frac{1}{\varepsilon} Q(f, f), \tag{9}$$

and the collision term is written as:

$$\begin{aligned} & \frac{1}{\varepsilon} Q(f, f) = \int_{-\infty}^{+\infty} \int_0^{4\pi} \sigma V_r [f^* f_1^* - f f_1] d\Omega dV_1 \\ &= \int_{-\infty}^{+\infty} \int_0^{4\pi} \sigma V_r f^* f_1^* d\Omega dV_1 - f \int_{-\infty}^{+\infty} \int_0^{4\pi} \sigma V_r f_1 d\Omega dV_1 \\ &= \frac{1}{\varepsilon} [P(f, f) - \mu(\mathbf{V})f] \end{aligned} \tag{10}$$

Where,

$$\mu(\mathbf{V}) = \int_{-\infty}^{+\infty} \int_0^{4\pi} \sigma V_r f_1 d\Omega dV_1 = \int_0^{4\pi} \sigma V_r d\Omega \int_{-\infty}^{+\infty} f_1 dV_1 = \kappa \rho / m$$

is the mean collision frequency for the molecules having velocity \mathbf{V} , ρ is the density of the gas, m is the mass of a molecule of the gas, κ is a molecular constant $\kappa = \int_0^{4\pi} \sigma V_r d\Omega$ and $\rho/m = \int_{-\infty}^{+\infty} f_1 dV_1$ (Wild, 1951). In a special case in which σV_r is independent of V_r (Maxwellian molecules), we have:

$$\mu(\mathbf{V}) = \mu = \frac{\kappa \rho}{m} \tag{11}$$

Substituting Eqs. (10) and (11) into Eq. (9):

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon} Q(f, f) = \frac{1}{\varepsilon} [P(f, f) - \mu f] \tag{12}$$

The first-order time discretization of Eq. (12) is written as:

$$\frac{f^{n+1} - f^n}{\Delta t} = \frac{1}{\varepsilon} [P(f^n, f^n) - \mu f^n] \tag{13}$$

$$f^{n+1} = \left(1 - \frac{\mu \Delta t}{\varepsilon}\right) f^n + \frac{\mu \Delta t}{\varepsilon} \frac{P(f^n, f^n)}{\mu}$$

The probabilistic interpretation of Eq. (13) is the following. In order a particle is sampled from f^{n+1} , a particle is sampled from f^n , with probability of $(1 - \mu \Delta t / \varepsilon)$ and a particle is sampled from $P(f^n, f^n) / \mu$, with probability of $\mu \Delta t / \varepsilon$. However, the above probabilistic interpretation fails if the ratio of $\mu \Delta t / \varepsilon$ is too large because the coefficient of f^n on the right hand side may become negative. This means that in the stiff region (where the Knudsen number is small $\varepsilon \ll 1$) the time step becomes extremely small; therefore, the method becomes almost unstable near the fluid regime [15, 16].

To circumvent the problem, a new independent variable τ and a new dependent variable $F(V, \tau)$ are defined as:

$$\tau = (1 - e^{-\mu t / \varepsilon}) \tag{14}$$

$$F(V, \tau) = f(V, t) e^{\mu t / \varepsilon} \tag{15}$$

Therefore, Eq. (12) is rewritten as:

$$\frac{\partial F}{\partial \tau} = \frac{1}{\mu} P(F, F) \tag{16}$$

$$F(V, \tau = 0) = f(V, 0)$$

Eq. (16) is the Cauchy problem, and it has a power series solution as follows [14]:

$$\frac{\partial F}{\partial \tau} = \frac{1}{\mu} P(F, F) \tag{17}$$

$$F(V, \tau = 0) = f(V, 0)$$

Substituting Eq. (17) into Eq. (16):

$$\frac{\partial F}{\partial \tau} = \sum_{k=0}^{\infty} k \tau^{k-1} f_k = \sum_{k=0}^{\infty} (k+1) \tau^k f_{k+1} \tag{18}$$

$$P(F, F) = P\left(\sum_{k=0}^{\infty} \tau^k f_k, \sum_{k=0}^{\infty} \tau^k f_k\right)$$

Expanding the summation terms:

$$\frac{\partial F}{\partial \tau} = f_1 + 2\tau f_2 + 3\tau^2 f_3 + 4\tau^3 f_4 + \dots \tag{19}$$

$$P(F, F) = P(f_0 + \tau f_1 + \tau^2 f_2 + \dots, f_0 + \tau f_1 + \tau^2 f_2 + \dots)$$

Substituting Eq. (19) into Eq. (16):

$$f_1 + 2\tau f_2 + 3\tau^2 f_3 + 4\tau^3 f_4 + \dots = \frac{1}{\mu} P(f_0 + \tau f_1 + \tau^2 f_2 + \dots, f_0 + \tau f_1 + \tau^2 f_2 + \dots) \tag{20}$$

$$= \frac{1}{\mu} \left[P(f_0, f_0) + \tau P(f_0, f_1) + \tau P(f_1, f_0) + \tau^2 P(f_0, f_2) + \tau^2 P(f_2, f_0) + \tau^2 P(f_1, f_1) + \dots \right]$$

$$= \frac{1}{\mu} \left[P(f_0, f_0) + 2\tau P(f_0, f_1) + 2\tau^2 P(f_0, f_2) + \tau^2 P(f_1, f_1) + \dots \right]$$

$$= \frac{1}{\mu} \left[P(f_0, f_0) + 2\tau P(f_0, f_1) + \tau^2 \{2P(f_0, f_2) + P(f_1, f_1)\} + \dots \right]$$

Equating the coefficients of corresponding powers of τ , we can find for f as:

$$f_1 = \frac{1}{\mu} P(f_0, f_0)$$

$$f_2 = \frac{1}{\mu} P(f_0, f_1) \tag{21}$$

$$f_3 = \frac{1}{\mu} \left\{ \frac{2}{3} P(f_0, f_2) + \frac{1}{3} P(f_1, f_1) \right\}$$

$$\vdots$$

Therefore, the function f is found by the recurrence formula as:

$$f_{k+1} = \frac{1}{k+1} \sum_{h=0}^k \frac{1}{\mu} P(f_h, f_{k-h}) \tag{22}$$

$$k = 0, 1, \dots$$

Converting Eq. (17) into original variables we obtain the following formula representing the solution to the Cauchy problem 9:

$$f(v, t) = e^{-\mu t / \varepsilon} \sum_{k=0}^{\infty} (1 - e^{-\mu t / \varepsilon})^k f_k(v) \tag{23}$$

A class of numerical schemes based on a suitable

truncation for $m \geq 1$ of Eq. (23) is derived [14]:

$$f(v, t) = e^{-\mu t/\varepsilon} \sum_{k=0}^m (1 - e^{-\mu/\varepsilon})^k f_k(v) + (1 - e^{-\mu/\varepsilon})^{m+1} M(v). \tag{24}$$

Where $f^n = f(n\Delta t)$ and Δt is time step. The quantity M in Eq. (24) is the asymptotic solution of the equation and called Maxwellian. Eq. (24) can be generalized by using different weight functions including the influence of the higher order coefficients. In general the TRMC scheme is written as:

$$f^{n+1} = \sum_{k=0}^m A_k f_k + A_{m+1} M. \tag{25}$$

Where, the functions f_k are given by Eq. (22) and the weight functions $A_k(\tau)$ are non-negative functions that satisfy the consistency, conservative and the asymptotic preservation condition (Gabetta et al., [14]). In this simulation the first order TRMC of Eq. (25) as $f^{n+1} = A_0 f_0^n + A_1 f_1 + A_2 M$ is used.

3. Analytical solutions

The energy E of a particle in an axially symmetric gas mixture flow inside a rotating cylinder is given as [17],

$$E(r) = \frac{1}{2} I \omega^2 = \frac{1}{2} m r^2 \omega^2. \tag{26}$$

The rotational effect is the same as additional external field acting on the system and may be written as:

$$U(r) = -\frac{1}{2} m r^2 \omega^2. \tag{27}$$

Using the Boltzmann distribution for the particle number density and substituting for $U(r)$ from Eq. (27):

$$n(r) = A \exp\left(-\frac{U(r)}{kT}\right) = A \exp\left(\frac{m r^2 \omega^2}{2kT}\right) \tag{28}$$

Where the normalization factor A can be determined by $N = \int n(r) dV$ giving:

$$N = \int_0^R \int_0^{2\pi} A \exp\left(-\frac{U(r)}{kT}\right) r dr d\theta \tag{29}$$

$$= \int_0^R \int_0^{2\pi} A \exp\left(\frac{m r^2 \omega^2}{2kT}\right) r dr d\theta,$$

$$N = 2\pi A \int_0^R \exp\left(\frac{m r^2 \omega^2}{2kT}\right) r dr =$$

$$\pi A \int_0^R \exp\left(\frac{m r^2 \omega^2}{2kT}\right) d(r^2) \tag{30}$$

$$= \pi A \frac{2kT}{m\omega^2} \exp\left(\frac{m r^2 \omega^2}{2kT}\right) \Big|_0^R$$

$$= \frac{2\pi A kT}{m\omega^2} \left(\exp\left(\frac{m R^2 \omega^2}{2kT}\right) - 1 \right).$$

Then for A can be written:

$$A = \frac{Nm\omega^2}{2\pi kT} \left(\exp\left(\frac{m R^2 \omega^2}{2kT}\right) - 1 \right)^{-1}. \tag{31}$$

Therefore:

$$n(r) = \frac{Nm\omega^2}{2\pi kTL} \cdot \frac{\exp\left(\frac{m\omega^2 r^2}{2kT}\right)}{\exp\left(\frac{m\omega^2 R^2}{2kT}\right) - 1}. \tag{32}$$

Where, N is the total number of molecules, m is the mass of a molecule of gas, ω is the angular velocity, k is the Boltzmann constant, T is the absolute temperature, L is the length of the cylinder, R is the cylinder radius and r is the radial distance.

4. Boundary and initial conditions

4.1 Boundary conditions

At the boundary where the axis of symmetry exists the rule of specular reflection is considered. The specular reflection rule is implemented for molecules at the solid surface boundary with normal velocity to the solid boundary being reversed and those with parallel velocity to the solid surface boundary remaining unchanged. At the top and the bottom boundary of the cylinder the rule of specular reflection and at the wall of the cylinder the rule of diffusion reflection are considered. The diffuse reflection rule is implemented for molecules at the solid surface boundary with a velocity component equal to the tangential

velocity at the cylinder wall equal to 1000 meter/second and the other component of the velocity is equal to the most probable velocity according to the equilibrium Maxwellian distribution. Therefore, the resultant velocity is equal to the velocity that was obtained in accordance with the kinetic theory of gases. In the diffuse reflection rule the temperature of the reflected molecule and the temperature of the solid wall boundary are required to be equal, and the velocities of the reflected molecules are distributed according to equilibrium Maxwellian distribution.

4.2 Initial conditions

The initial values of the gas mixture pressure and the temperature are 2.76 Pascal absolute and 200 Kelvin, respectively. The molar concentrations of the gas mixture inside the cylinder consist of 50% argon and 50% helium. The initial velocities of the molecules are obtained based on the kinetic theory.

5. The Numerical procedures

In the simulation of the problem using the DSMC method, two grid systems are chosen. The first grid system (Fig. 1) is used to calculate the averaging of flow properties. This grid system is chosen to be fine enough in order to increase our computational accuracy. The grid system is refined up to where the variations of the flow properties are not substantial (the variations of the flow properties less than 2%). The second grid system is chosen to be very fine (the mesh size is equal to 0.2 times the mean free path of the molecules); therefore, the collisions of the molecules are controlled within each mesh accurately. Our grid system consists of 5 times 100 meshes and the total number of model molecules is 35700. The number of real molecules is obtained based on the gas density and Avogadro's number where each model molecule consists of 5.49735×10^{15} real molecules. In the TRMC scheme the same grid system (5 times 100) and the same number of model molecules, 35700, are used. The number of real molecules is

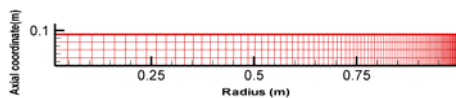


Fig. 1. The structure of mesh system for the cylinder of radius 1 meter and height of 0.1 meter.

obtained based on the density of gas and Avogadro's number. For the axially symmetric flows, the distribution of the modeled molecules is linearly proportional to the radial distance. The volume of the mesh far from the axis of symmetry is much larger than the volume of the mesh close to the axis of symmetry. Therefore, the number of the modeled molecules far from the axis of symmetry is much greater than the number of modeled molecules close to the axis of symmetry. This leads to the uniformity of density in the radial direction. The size of the mesh is on the order of the mean free path, and the time step in our simulation is chosen to be 0.2 times the mean collision time Bird [1]. The molecules are distributed in the mesh system according to the normal distribution. The initial velocity of the molecules is chosen based on the kinetic theory of gases. The direction of velocity of the molecules is chosen randomly based on equilibrium Maxwellian distribution. We then start to advance with time and the new position of the molecules is designated. The collisions of the model molecules are done based on the variable hard sphere (VHS) model proposed by Bird [1]. We then continue advancing in time until the statistical fluctuations of the flow properties are minimum. In the simulation of gas mixture (argon and helium) the flow inside the high speed rotating cylinder the gas mixture pressure inside the cylinder is initially 2.76 Pascal absolute, the radius of the cylinder is 1 meter, the tangential velocity at the cylinder wall is 1000 meter/second, the gas mixture inside the cylinder consists of 50% argon and 50% helium, and the temperature of the gas mixture inside the cylinder is 200 Kelvin. The total number of 35700 model molecules is considered to be distributed linearly along the radial coordinates. The time-step of the simulation is chosen to be 10^{-6} second and the simulation is done until 25.7 seconds of real time (1280000 iterations) in DSMC method. In the TRMC scheme the time-step of the simulation is chosen to be 5×10^{-6} second and the simulation is done until 25.7 seconds of real time (256000 iterations). The calculations are performed by an IBM compatible personal computer with 2.8 GHz CPU and 512 MB RAM.

5.1 Algorithm of the Direct Simulation Monte Carlo Method (DSMC)

DSMC Algorithm (for the VHS collision model molecules).

- $T_{ref} = 273K$

- $d_{p_{ref}} = 2.33 \times 10^{-10}$, for He
- $d_{q_{ref}} = 4.17 \times 10^{-10}$, for Ar
- $m_r = m_p m_q / m_p + m_q$
- $k = 1.380658 \times 10^{-23} J K^{-1}$
- $\Delta t = 1 \times 10^{-6} Sec$
- Distribute the initial locations of the particles according to the uniform distribution.
- for $n_i = 1$ to n_{tot}
 - Given $\{v_i^n, i = 1, \dots, N\}$.
 - Define the local Knudsen number (ε).
 - Calculate

$$d_{pq} = \left(d_{ref} \right)_{pq} \left[\frac{\left\{ 2k(T_{ref})_{pq} / \left(m_r |\mathbf{v}_i - \mathbf{v}_j|^2 \right) \right\}^{\gamma_{pq} - 1/2}}{\Gamma(5/2 - \gamma_{pq})} \right].$$

- Compute an upper bound $\bar{\sigma} = \max((\pi/4)d_{pq}^2(|\mathbf{v}_i - \mathbf{v}_j|))$ for the cross section, $\bar{\sigma}$ is updated in each collision.
- Set $\mu = 4\pi\bar{\sigma}$.
- Set $N_c = Iround(\mu N \Delta t / (2\varepsilon))$.
- Select $2N_c$ dummy collision pairs (i, j) uniformly among all possible pairs, and for those.
- Compute the relative cross-section $\sigma_{ij} = (\pi/4)d_{pq}^2|\mathbf{v}_i - \mathbf{v}_j|$.
- Generate uniform random numbers (Rand).
- if $Rand < \sigma_{ij}/\bar{\sigma}$
 - Perform the collision between i and j , and compute the post-collision velocities \mathbf{v}_i^* and \mathbf{v}_j^* according to the collisional law.
 - Generate two uniform random numbers ξ_1, ξ_2 .
 - Set $\alpha = \cos^{-1}(2\xi_1 - 1)$, $\beta = 2\pi\xi_2$.
 - Set $\phi = (\cos\beta \sin\alpha \quad \sin\beta \sin\alpha \quad \cos\alpha)^T$.
 - $\mathbf{v}_i^* = \frac{1}{2}(\mathbf{v}_i + \mathbf{v}_j) + \frac{1}{2}|\mathbf{v}_i - \mathbf{v}_j|\phi$,
 - Set $\mathbf{v}_j^* = \frac{1}{2}(\mathbf{v}_i + \mathbf{v}_j) - \frac{1}{2}|\mathbf{v}_i - \mathbf{v}_j|\phi$.
 - Set $\mathbf{v}_i^{n+1} = \mathbf{v}_i^*$, $\mathbf{v}_j^{n+1} = \mathbf{v}_j^*$.
- else
 - Set $\mathbf{v}_i^{n+1} = \mathbf{v}_i^n$, $\mathbf{v}_j^{n+1} = \mathbf{v}_j^n$.
 - Set $\mathbf{v}_i^{n+1} = \mathbf{v}_i^n$ for the $N_i - 2N_c$ particles that have not been selected.
- End for
- Calculate macroscopic properties:
- macroscopic flow velocity: $\bar{\mathbf{v}}_0 = \frac{1}{\rho} (m_p n_p \bar{\mathbf{v}}_p + m_q n_q \bar{\mathbf{v}}_q)$,
- density: $\rho = n m$,
- thermal Velocity: $\mathbf{v}'_i = \bar{\mathbf{v}}_i - \bar{\mathbf{v}}_0$,

- temperature: $T_{tr} = \frac{1}{3kn} (n_p m_p v_p'^2 + n_q m_q v_q'^2)$,
- pressure: $P = nkT_{tr} = \frac{1}{3} (n_p m_p v_p'^2 + n_q m_q v_q'^2)$.

During each step, all the other $N_i - 2N_c$ particle velocities remain unchanged.

Here, by $Iround(x)$, we denote a suitable integer rounding of a positive real number x .

In our algorithm, we choose:

$$Iround(x) = \begin{cases} [x] & \text{with probability } [x] + 1 - x \\ [x] + 1 & \text{with probability } x - [x] \end{cases}$$

5.2 Algorithm of the Time Relaxed Monte Carlo Method (TRMC)

TRMC Algorithm (first order TRMC scheme for the VHS collision model molecules).

- $T_{ref} = 273K$
 - $d_{p_{ref}} = 2.33 \times 10^{-10}$, for He
 - $d_{q_{ref}} = 4.17 \times 10^{-10}$, for Ar
 - $m_r = m_p m_q / m_p + m_q$
 - $k = 1.380658 \times 10^{-23} J K^{-1}$
 - $\Delta t = 1 \times 10^{-6} Sec$
 - Distribute the initial locations of the particles according to the uniform distribution.
 - for $n_i = 1$ to n_{tot}
 - Given $\{v_i^n, i = 1, \dots, N\}$.
 - Define the local Knudsen number (ε).
 - Calculate
- $$d_{pq} = \left(d_{ref} \right)_{pq} \left[\frac{\left\{ 2k(T_{ref})_{pq} / \left(m_r |\mathbf{v}_i - \mathbf{v}_j|^2 \right) \right\}^{\gamma_{pq} - 1/2}}{\Gamma(5/2 - \gamma_{pq})} \right].$$
- Compute an upper bound $\bar{\sigma} = \max((\pi/4)d_{pq}^2(|\mathbf{v}_i - \mathbf{v}_j|))$ for the cross section, $\bar{\sigma}$ is updated in each collision.
 - Set $\tau = 1 - \exp(-\rho\bar{\sigma}\Delta t / \varepsilon)$.
 - Compute $A_1(\tau) = \tau^2 - \tau^3$, $A_2(\tau) = \tau^3 - \tau^4$
 - Set $N_c = Iround(N A_1 / 2)$.
 - Select N_c dummy collision pairs (i, j) uniformly among all possible pairs.
 - Compute the relative cross-section $\sigma_{ij} = (\pi/4)d_{pq}^2|\mathbf{v}_i - \mathbf{v}_j|$.
 - Generate uniform random numbers (Rand).
 - if $Rand < \sigma_{ij}/\bar{\sigma}$
 - Perform the collision between i and j , and

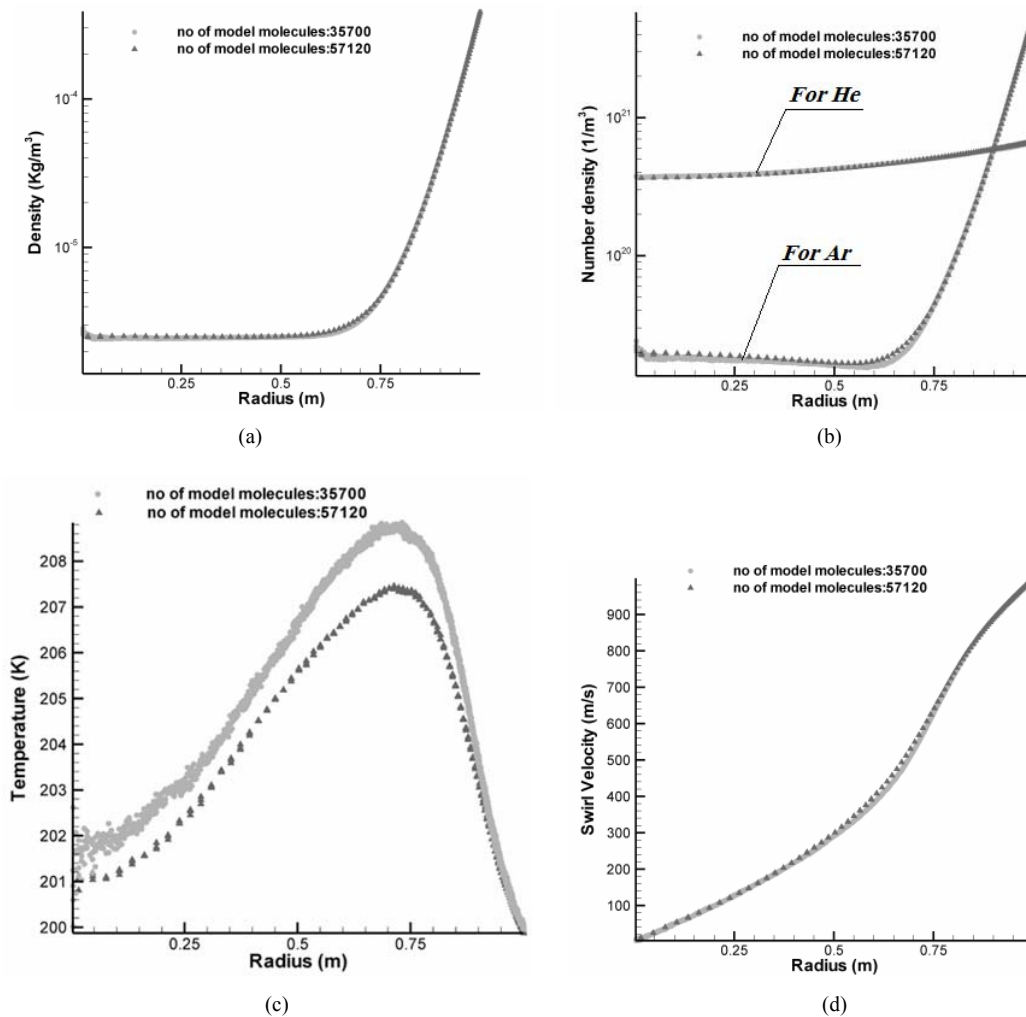


Fig. 2. Number of molecules dependency test: (a) Density, (b) Number density, (c) Temperature, (d) Swirl velocity.

compute the post-collision velocities \mathbf{v}_i^* and \mathbf{v}_j^* according to the collisional law.

- Generate two uniform random numbers ξ_1, ξ_2 .

- Set $\alpha = \cos^{-1}(2\xi_1 - 1), \beta = 2\pi\xi_2$.

- Set $\phi = (\cos\beta \sin\alpha \quad \sin\beta \sin\alpha \quad \cos\alpha)^T$.

$$\mathbf{v}_i^* = \frac{1}{2}(\mathbf{v}_i + \mathbf{v}_j) + \frac{1}{2}|\mathbf{v}_i - \mathbf{v}_j|\phi,$$

- Set

$$\mathbf{v}_j^* = \frac{1}{2}(\mathbf{v}_i + \mathbf{v}_j) - \frac{1}{2}|\mathbf{v}_i - \mathbf{v}_j|\phi$$

- Set $\mathbf{v}_i^{n+1} = \mathbf{v}_i^*, \mathbf{v}_j^{n+1} = \mathbf{v}_j^*$.

◦ else

- Set $\mathbf{v}_i^{n+1} = \mathbf{v}_i^n, \mathbf{v}_j^{n+1} = \mathbf{v}_j^n$.

- Set $\mathbf{v}_i^{n+1} = \mathbf{v}_i^n$ for the $N_i - 2N_c$ particles that have not been selected.

- Set $N_M = \text{Iround}(NA_2)$.

- Select N_M particles among those that have not collided, and compute their mean momentum and energy.

- Sample N_M particles from the Maxwellian with the above momentum and energy, and replace the N_M selected particles with the sampled ones.

◦ Set $\mathbf{v}_i^{n+1} = \mathbf{v}_i^n$ for all the $N - 2N_c - N_M$ particles that have not been selected.

• End for

- Calculate macroscopic properties:
- macroscopic flow velocity:

$$\bar{v}_0 = \frac{1}{\rho} (m_p n_p \bar{v}_p + m_q n_q \bar{v}_q),$$

- density: $\rho = n.m$,
- thermal Velocity: $v'_i = \bar{v}_i - \bar{v}_0$,
- temperature: $T_{tr} = \frac{1}{3kn} (n_p m_p v_p'^2 + n_q m_q v_q'^2)$,
- pressure: $P = nkT_{tr} = \frac{1}{3} (n_p m_p v_p'^2 + n_q m_q v_q'^2)$.

6. The Number of model molecules dependency test

The number of model molecules dependency test is done by using more model molecules in each mesh. The simulation is performed by using 35700 model molecules in the grid system; however, in the number of model molecules dependency test the number of model molecules is increased to 57120 in our grid system. The results of simulation of flow characteristics for the two cases (35700 model molecules and 57120 model molecules in the grid system) at 4 seconds of real time of flow simulation are obtained and compared with each other. Figs. 2(a), 2(b), 2(c) and 2(d) show the number of molecules dependency test for density, number density, temperature and swirl velocity, respectively. Fig. 2(a) shows the number of model molecules dependency test for the mixture density. The maximum discrepancy between the results of the simulation of the number of model molecules dependency test for the mixture density for the two cases (35700 model molecules and 57120 model molecules in the grid system) is less than 4% at 0.625 meter of radial distance inside the cylinder. Fig. 2(b) shows the number of model molecules dependency test for number densities of argon and helium. The maximum discrepancy between the results of simulation of number of model molecules dependency test for the number density of argon and helium for the two cases (35700 model molecules and 57120 model molecules in the grid system) is less than 7.3% at 0.625 meter of radial distance inside the cylinder and less than 1.35% at 0.1 meter of the radial distance inside the cylinder, respectively. Fig. 2(c) shows the number of model molecules dependency test for the temperature. The maximum discrepancy between the results of simulation of the number of model molecules dependency test for the temperature for the two

cases (35700 model molecules and 57120 model molecules in the grid system) is less than 0.66% at 0.75 meter of radial distance inside the cylinder. Fig. 2d shows the number of model molecules dependency test for the swirl velocity. The maximum discrepancy between the results of simulation of number of model molecules dependency test for the swirl velocity for the two cases (35700 model molecules and 57120 model molecules in the grid system) is less than 4.37% at 0.625 meter of radial distance inside the cylinder.

7. Discussion of results

Fig. 3(a) shows the comparison of the results of simulations using the DSMC method and the TRMC scheme with the results of Bird, [1] for the variations of the swirl velocity along the radial coordinates. Comparison of our results of simulation using the DSMC method for the swirl velocity with the results of Bird [1] shows good agreement at 0.2 second of real time (10000 iterations); however, comparisons of our results of simulations using the DSMC method at 25.7 seconds of real time (1280000 iterations) and the results of simulation using the TRMC scheme at 25.7 seconds of real time (256000 iterations) with the results of Bird, [1] show high discrepancies. The discrepancies are due to the lack of sufficient real time (number of iterations) in the calculation of the Bird [1] simulation. In that simulation the DSMC method is used; however, larger time-steps are not allowed [12]; therefore, one is not able to reach the stationary flow simulation. Comparisons of our results of simulation using the DSMC method at 25.7 seconds of real time (1280000 iterations) for the swirl velocity with the results of simulation using the TRMC scheme at 25.7 seconds of real time (256000 iterations) show good agreement. Fig. 3(b) shows the time evolution of the variations of swirl velocity along the radial coordinates for different iterations (10000 to 1280000 iterations). Fig. 4(a) shows the comparison of the results of simulations using the DSMC method and the TRMC scheme with the results of Bird [1] for the variations of the gas mixture (argon and helium) temperature along the radial coordinates. Comparison of the results of simulation using the DSMC method for the gas mixture (argon and helium) temperature with the results of Bird, [1] shows good agreement at 0.2 second of real time (10000 iterations). However, comparisons of our results of simulations using the

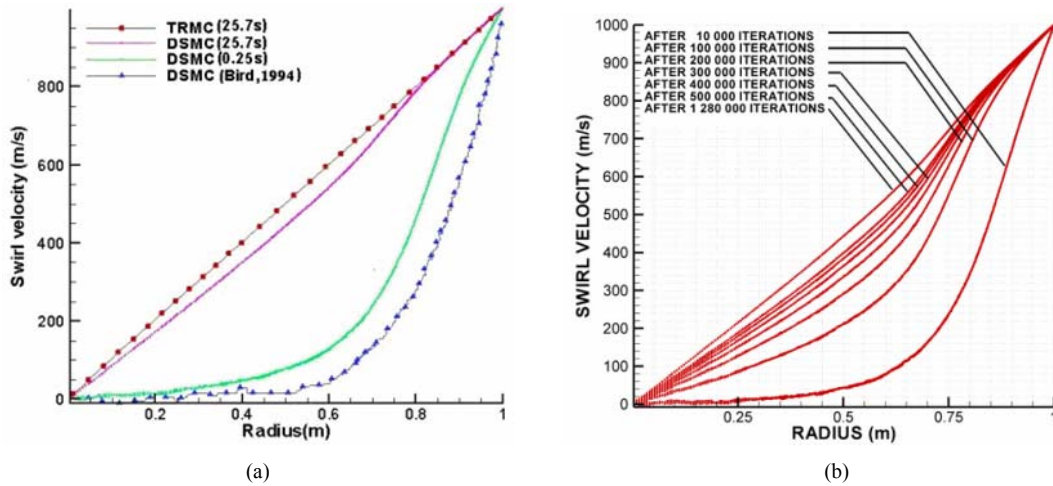


Fig. 3. Swirl velocity: (a) Comparison between the results of simulation using the DSMC method, the TRMC scheme and the results of Bird, 1994 for the variations of the swirl velocity along the radial coordinates, (b) Time evolution of the variations of swirl velocity along the radial coordinates from the 0.25 second of real time (12500 iterations) up to 25.7 seconds of real time (1280000 iterations).

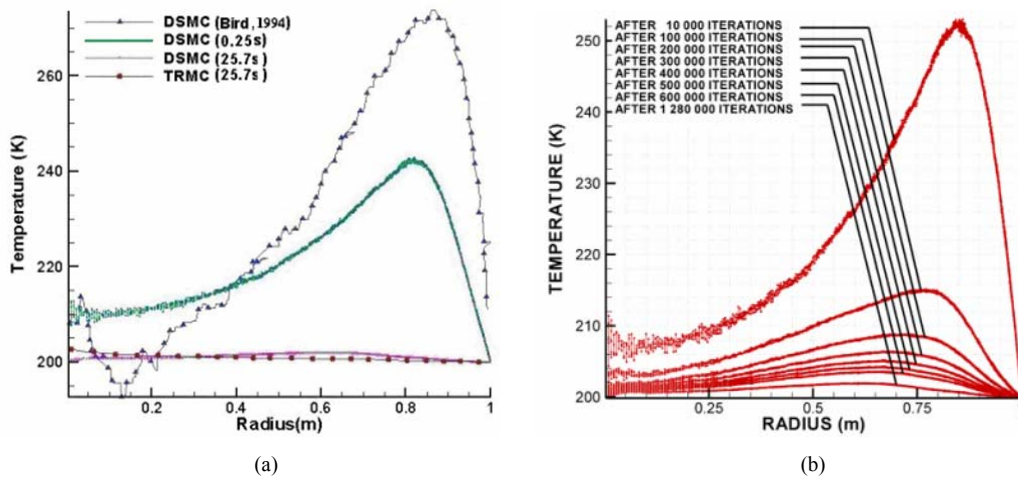


Fig. 4. Temperature: (a) Comparison between the results of simulation using the DSMC method, the TRMC scheme and the results of Bird, 1994 for the variations of the temperature along the radial coordinates, (b) Time evolution of the variations of temperature along the radial coordinates from the 0.25 second of real time (12500 iterations) up to 25.7 seconds of real time (1280000 iterations).

DSMC method at 25.7 seconds of real time (1280000 iterations) and the results of simulation using the TRMC scheme at 25.7 seconds of real time (256000 iterations) with the results of Bird, [1] show high discrepancies. The discrepancies are due to the lack of sufficient real time of computing (number of iterations) in the Bird, [1] calculations. This is because in the Bird calculations using the DSMC method one is unable to choose larger time steps; however, in the simulation using the TRMC scheme one is allowed to

choose larger time-steps (see [12]), therefore reaching larger real time for calculations. Comparisons of our results of simulation using the DSMC method at 25.7 seconds of real time (1280000 iterations) for the gas mixture (argon and helium) temperature with the results of simulation using the TRMC scheme at 25.7 seconds of real time (256000 iterations) show good agreement. Fig. 4(b) shows the time evolution of the variations of the gas mixture (argon and helium) temperature along the radial coordinates for different

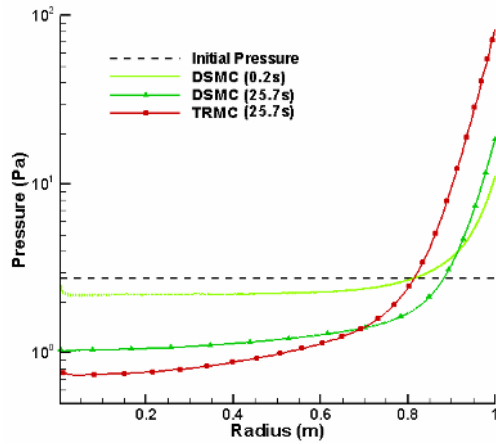


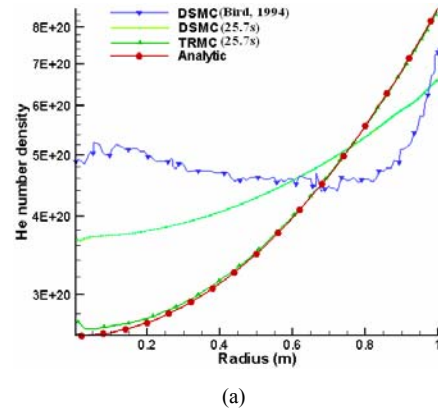
Fig. 5. Comparison between the results of simulations using the DSMC method, the TRMC scheme for the variations of the gas mixture (argon and helium) pressure along the radial coordinates.

iterations (10000 to 1280000 iterations). Fig. 5 shows the comparison of the results of simulations using the DSMC method with the TRMC scheme for the variations of the gas mixture (argon and helium) pressure along the radial coordinates. Fig. 5 shows that at 25.7 seconds of real time (1280000 iterations) the values of pressure around the wall of the cylinder are approximately 18 times bigger than the values of pressure around the center of the cylinder.

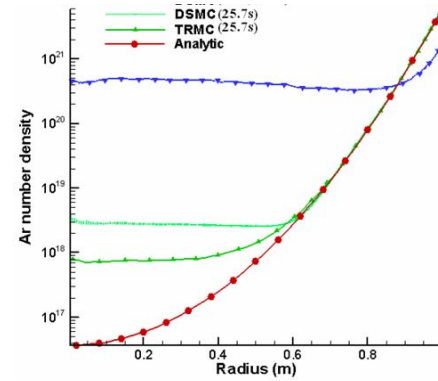
7.1 Comparisons of number density results with the analytical solution

The analytical solution of Kuo [17] is only used here as a reference to make the comparison of the results of the present simulation, since the solution of Kuo [17] is based on the assumption that the flow is in equilibrium. Here in the present simulation one assumes that the results of our simulation reached the equilibrium condition as well. However, this assumption is not completely valid. Therefore, the analytical solution of Kuo [17] can only be used as a reference and not as an absolute source to judge the accuracy of the TRMC scheme.

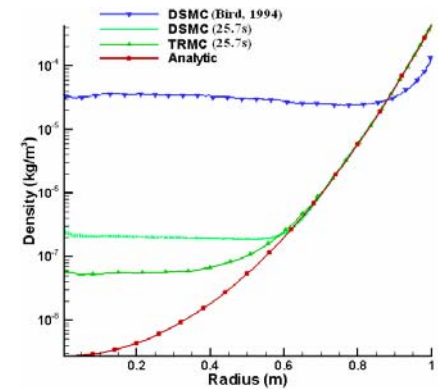
Figs. 6(a), 6(b) and 6(c) show the comparisons between the DSMC method, the TRMC scheme and the results of Bird [1] with the analytical solution for the variations of the density of gas mixture, the number density of helium and the number density of argon along the radial coordinates, respectively. Comparison of our results of simulation for the density of the gas mixture [Fig. 6(a)] with the analytical solution



(a)



(b)



(c)

Fig. 6. He number density, Ar number density and Density: (a) Comparison between the DSMC scheme, the TRMC scheme and the results of Bird 1994 with the analytical solution for the variations of the number density of helium along the radial coordinates, (b) Comparison between the DSMC scheme, the TRMC scheme and the results of Bird 1994 with the analytical solution for the variations of the number density of Argon along the radial coordinates, (c) Comparison between the DSMC scheme, the TRMC scheme and the results of Bird 1994 with the analytical solution for the variations of the density along the radial coordinates.

shows reasonable agreement, and the agreement is pronounced for the radial distance of $r > 0.5m$; however, the comparison of our results of simulation using the DSMC and the TRMC with the analytical solution shows better agreement than the results of Bird, [1] [Fig. 6(a)]. Comparison of our results of simulation for the number density of helium [Fig. 6(b)] with the analytical solution shows reasonable agreement, and the agreement is pronounced for a radial distance of $r > 0.5m$. However, comparison of the results of simulation of Bird, [1] for the number density of helium [Fig. 6(b)] with the analytical solution shows high discrepancies. The discrepancies of the Bird results are due to the lack of sufficient real time in the simulation using the DSMC method. In the simulation using the DSMC method, one is not allowed to choose larger time-steps; therefore, reaching the larger real time is very difficult. However, in the simulation using the TRMC scheme, one is allowed to choose larger time-steps in order to reach larger real time. Comparison of our results of simulation for the number density of argon [Fig. 6(c)] with the analytical solution shows better agreement than the comparison of the results of simulation of Bird [1] for the number density of argon [Fig. 6(c)] with the analytical solution.

8. Conclusions

The comparison of the results of simulation using the DSMC method with the results of simulation using the TRMC scheme for the swirl velocity and the temperature show good agreement. However, the comparisons of the results for the swirl velocity and the temperature of Bird [1] with the analytical solution show high discrepancies. The comparisons of the results of simulations using the DSMC method and the TRMC scheme with the analytical solution for the density, number density of helium and number density of argon show good agreement. However, the comparisons of the results for the density, number density of Helium and number density of argon of Bird [1] show high discrepancies. The conclusions are summarized as follows:

Due to the required small time-steps in the DSMC simulations, the discrepancies of the results using the DSMC method are pronounced in comparison with the results of simulations using the TRMC scheme.

The comparisons of the results of simulations using the TRMC scheme for the density and the number

density with the analytical solution show better agreement than those obtained by DSMC method.

Having larger time-steps in the simulation using the TRMC scheme allows one to reach stationary results for the flow characteristics in shorter time; therefore, the results of simulations using the TRMC scheme show improvement over the results of simulations using the DSMC method. In the present simulation, there are two sources of approximation errors: the approximation errors inherent in the selection of larger time-step used in the TRMC scheme, and the approximation errors due to modeling the molecular collision, the VHS model, used in the present work. These two sources of approximation errors interact with each other. The nature of the interaction of the two sources of approximation errors is very complicated. However, the results of our simulation in the present work show that the approximation errors inherent in the selection of larger time-steps in the TRMC scheme counteract the other sources of approximation errors inherent in the simulation modeling, such as modeling of molecular collisions, the VHS model, used in the present work. Therefore the results of simulation, using the TRMC scheme, show improvement over the results of simulation using the DSMC method.

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