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Simulation of Rarefied Gas Between Coaxial Circular Cylinders by DSMC Method

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1. Introduction

In every system, if Knudsen number is larger than 0.1, the Navier-Stokes equation will not be satisfied for investigation of flow patterns. In this condition, the Boltzmann equation, presented by Ludwig Boltzmann in 1872, can be useful. The conditions that this equation can be used were investigted by Cercignani in 1969. The most successful method for solving Boltzmann equation for a rarefied gas system is Direct Simulation Monte Carlo (DSMC) method. This method was suggested by Bird in 1974. The cylindrical Couette flow and occurrence of secondry flow (Taylor vortex flow) in a annular domin of two coaxial rotating cylinders is a classical problem in fluid mechanics. Because this type of gas flow can occur in many industrical types of equipment used in chemical industries, Chemical engineers are interested in this problem. In 2000, De and Marino studied the effect of Knudsen number on flow patterns and in 2006 the effect of temperature gradient between two cylinders was investigated by Yoshio and his co-workers. The aim of the present paper is investigation of understanding of the effect of different conditions of rotation of the cylinders on the vortex flow and flow patterns.

2. Mathematical model

In the Boltzmann equation, the independent variable is the proption of molecules that are in a specific situation and dependent variables are time, velocity components and molecules positions. We consider the Boltzmann equation as follow:

$$\frac{\delta f}{\delta t}+\vec{v}.\frac{\delta f}{\delta \vec{x}}+\vec{F}.\frac{\delta f}{\delta \vec{v}}=\frac{1}{Kn}Q(f,f) \tag{1}$$

The bilinear collision operator, Q(f,f), describes the binary collosion of the particles and is given by:

$$Q(f,f)=\iint_{R^3 S^2}\sigma(\left|\vec{v}-\vec{v}_*\right|,\omega)(f'\ f'_*-ff_*)d\omega dv_* \tag{2}$$

Where, w is a unit vector of the shere S^2, so w is an element of the area of the surface of the unit sphere S^2 in R^3. With using this assumption that $\vec{f}$ is zero, we can rewrite equation 2 as:

$$Q(f,f)=\int_{R^3}\int_{S^2}\sigma(\left|\vec{v}-\vec{v}_*\right|,\omega)f'\,f_*'d\omega d\vec{v}_*-\int_{R^3}\int_{S^2}\sigma(\left|\vec{v}-\vec{v}_*\right|,\omega)ff_*d\omega d\vec{v}_* \tag{3}$$

The sign ′ is refered to values of distribution function after collision. The value of above integral is not related on $\vec{V}$, then we have

$$Q(f,f)=\int_{R^3}\int_{S^2}\sigma(\left|\vec{v}-\vec{v}_*\right|,\omega)f'\,f_*'d\omega d\vec{v}_*-f\int_{R^3}\int_{S^2}\sigma(\left|\vec{v}-\vec{v}_*\right|,\omega)f_*d\omega d\vec{v}_* \tag{4}$$

Inasmuch as the values of distribution function depend on its value before collision, we have:

$$Q(f,f)=P(f,f)-f\mu(\vec{v}) \tag{5}$$

Where $\mu(\vec{v})$ is the mean value of the collision of the particles that move with $\vec{v}$ velocity. Then we can estimate $\mu(\vec{v})$ as

$$\mu(\vec{v})=\mu=\frac{\kappa\rho}{m} \tag{6}$$

Then the Boltzmann equation can be written as

$$\frac{\delta f}{\delta t}+\vec{v}.\frac{\delta f}{\delta\vec{x}}=\frac{1}{Kn}\left[P(f,f)-f\mu(\vec{v})\right] \tag{7}$$

For solving this equation, we use fractional step method, so we have

$$\frac{\delta f}{\delta t}=-\vec{v}.\frac{\delta f}{\delta\vec{x}} \tag{8}$$

$$\frac{\delta f}{\delta t}=\frac{1}{Kn}Q(f,f)=\frac{1}{Kn}\left[P(f,f)-f\mu(\vec{v})\right] \tag{9}$$

Equation 8 describes the movement of the particles and equation 9 explains the collision of the particles. For estimation of new position of a mobile particle, we use following realationship

$$\vec{x}^{new}=\vec{x}^{old}+\vec{v}.\Delta t \tag{10}$$

For solving equation 9 by a numerical method, we can write it as

$$\frac{f^{n+1}-f^n}{\Delta t}=\frac{1}{Kn}\left[P(f^n,f^n)-\mu f^n\right] \tag{11}$$

If we rearrange it, we will have

$$f^{n+1}=\frac{\mu\Delta t}{Kn}.\frac{P(f^n,f^n)}{\mu}+(1-\frac{\mu\Delta t}{Kn})f^n \tag{12}$$

The first term on the right side of Eq. (12) is refered to probability of collision and the second term is refred to situation that no collision occurs.
Equation (12) is solved using the DSMC method. DSMC is a molecule-based statistical simulation method for rarefied gas introduced by Bird (2). It is a numerical solution method to solve the dynamic equation for gas flow by at least thousands of simulated molecules. Under the assumption of molecular chaos and gas rarefaction, the binary collisions are only considered. Therefore, the molecules' motion and their collisions are uncoupling if the computational time step is smaller than the physical collision time. After some steps, the macroscopic flow characteristics should be obtained statistically by sampling molecular properties in each cell and mean value of each property should be recorded. For estimation of macroscopic characteristics we used following realationship

$$\rho = \int_{\Re^3} f d\vec{v} \tag{13}$$

$$\rho\vec{u} = \int_{\Re^3} \vec{v} f d\vec{v} \tag{14}$$

$$T = \frac{1}{3\rho}\int_{\Re^3} \overline{(\vec{v}-\vec{u})} f d\vec{v} \tag{15}$$

$$p = \frac{\rho}{m} kT \tag{16}$$

3. Results and discussion

We consider a rarefied gas inside an annular domin of coaxial rotating cylinders. The radius of the inlet and the outlet cylinder are R1 and R2 (R1<R2). The bottom and top end of cylinders are covered with plates located at z=0 and z=L, repectively. Thus we consider a cylindrical domin R1<R2 ، $0 \le \Theta \le 2\pi$ and $0 \le z \le L$. Two cylinders are rotating around z-axes at surfac velocities $V_{\Theta 1}$ and $V_{\Theta 2}$ in the Θ direction. We will investigate the behavior of the gas numerically on the basis of Kinetic theory. The flow field is symmetric and the gas molecules are Hard-Sphere undergo diffuse reflection on the surface of the cylinders and specular reflection on the bottom and top boundaries. Here $Kn_0 = \lambda_0 / \Delta R$ is the Knudsen number with λ_0 being the mean free path of the gas molecules in the equilibrium state at rest with temerature T_0 and density ρ_0 . The distance between two cylinders is $\Delta R = R2 - R1$. In this work, R2/R1=2 and L/R1=1 and the number of cells are 100×100. The working gas was Argon, characterized by a specific haet ratio $\gamma = 5/3$. Considering as a Hard-Sphere gas the molecular diamete equal to $d = 4.17\times10^{-10} m$ and a molecular mass is $m = 6.63\times10^{-26} kgm^{-3}$ respectively.
Fig. 2 shows temperature contour when teperature of the inlet cylinder and the teperature of oulet cylinder are 300 and 350 K. Figs. 3 and 4 show flow field with a vortex flow. In Fig. 3, teperature of the inlet cylinder and the teperature of oulet cylinder are 300 and 350 K. In Fig. 4 teperature of the inlet cylinder and the teperature of oulet cylinder are 350 and 300 K. It can be seen that the direction of vortex in Fig. 3 is inverted in Fig. 4. Fig. 5 shows the

temperature plot at pressure 4, 40 and 400 Pa. It can be seen when the outlet cylinder is stagnant, the maximum amount of the temperature gradient occurs at the middle section and near the walls of the inlet cylinder. Fig. 6 shows density contour at pressure 4 Pa then maximum amount of density is near the walls of the outlet cylinder. Fig. 7 shows density contour at $V_{\Theta 1}/(2R\,T_0)^{1/2} = 0.26$ and $V_{\Theta 2}/(2R\,T_0)^{1/2} = 0.52$. Fig. 8 shows the flow field of single vortex flow at $V_{\Theta 1}/(2R\,T_0)^{1/2} = 0.81$ and $V_{\Theta 2}/(2R\,T_0)^{1/2} = -0.237$.

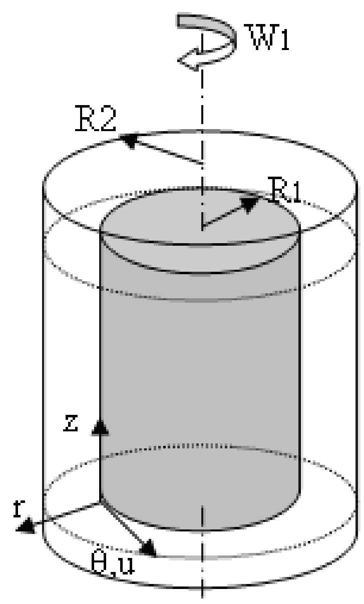

Fig. 1. Definition of the problem

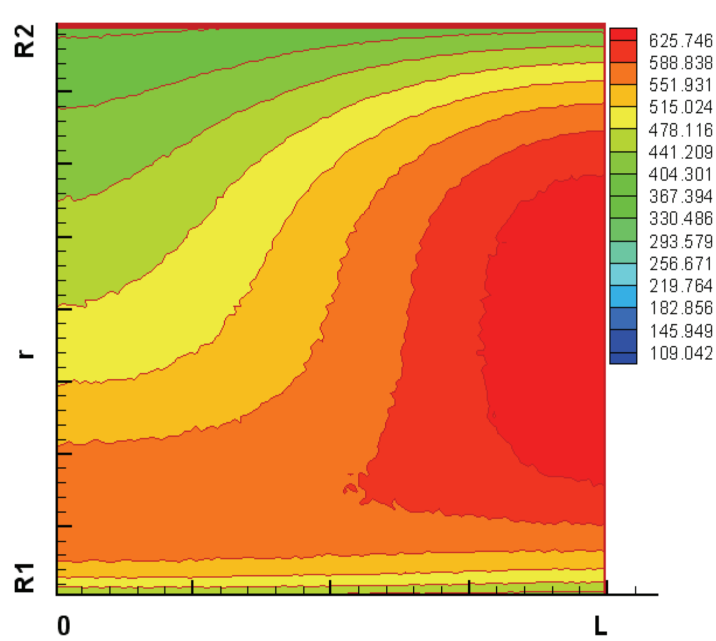

Fig. 2. Temperature contour when when teperature of the inlet cylinder and the teperature of oulet cylinder are 300 and 350 K

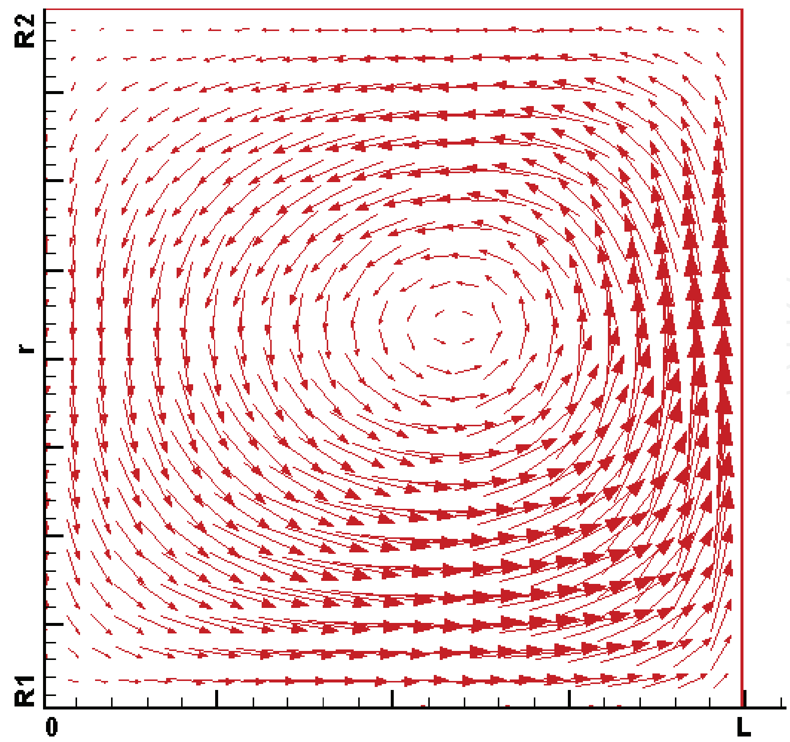

Fig. 3. Flow filed of single-vortex Flow when teperature of the inlet cylinder and the teperature of oulet cylinder are 300 and 350 K

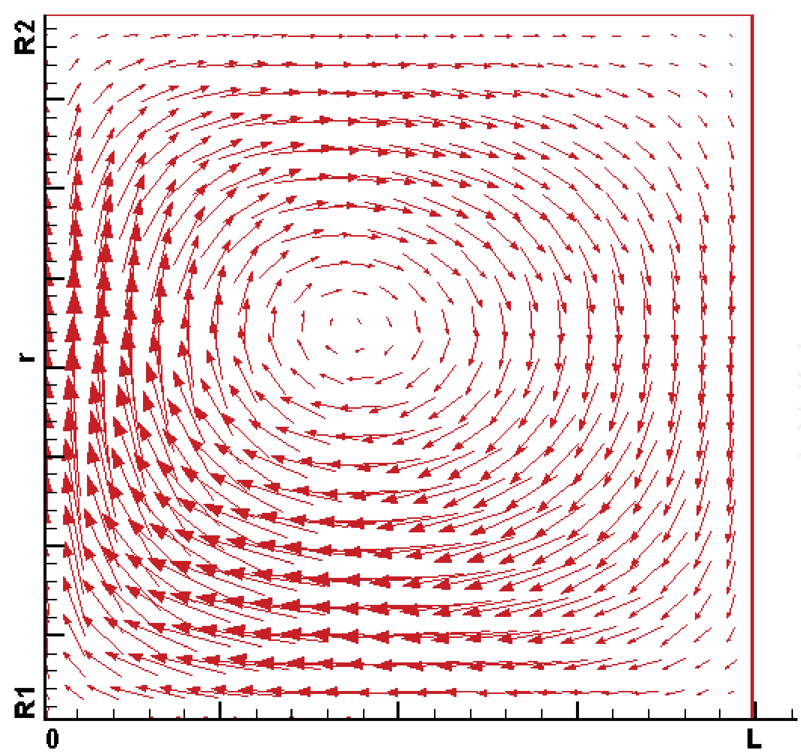

Fig. 4. Flow filed of single-vortex Flow when teperature of the inlet cylinder and the teperature of oulet cylinder are 350 and 300 K

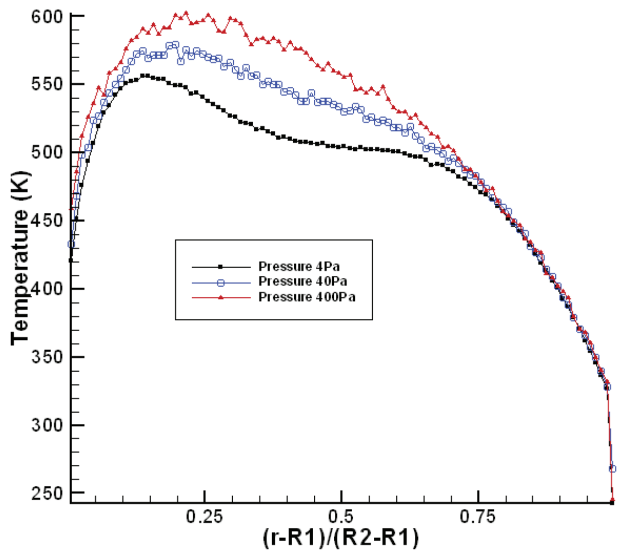

Fig. 5. Temperature at 4, 40 and 400 Pa

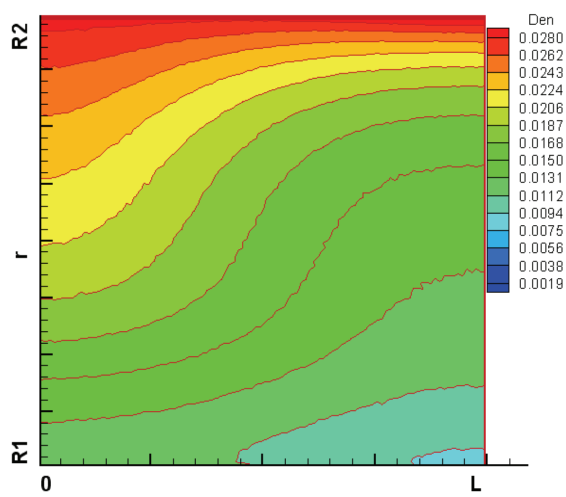

Fig. 6. Density contour at 4 Pa

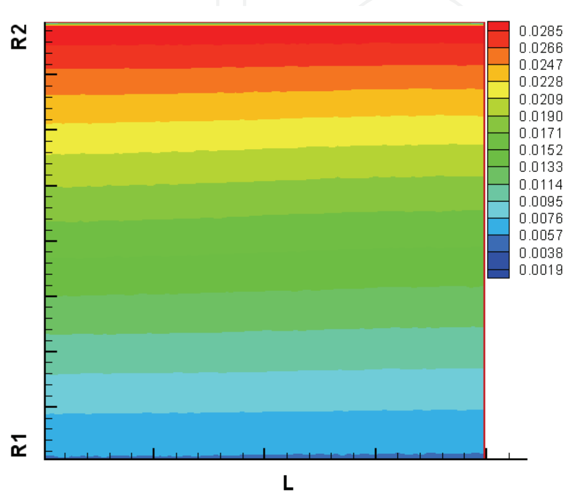

Fig. 7. Density contour at $V_{\Theta 1} / (2R\,T_0)^{1/2} = 0.26$ $V_{\Theta 2} / (2R\,T_0)^{1/2} = 0.52$

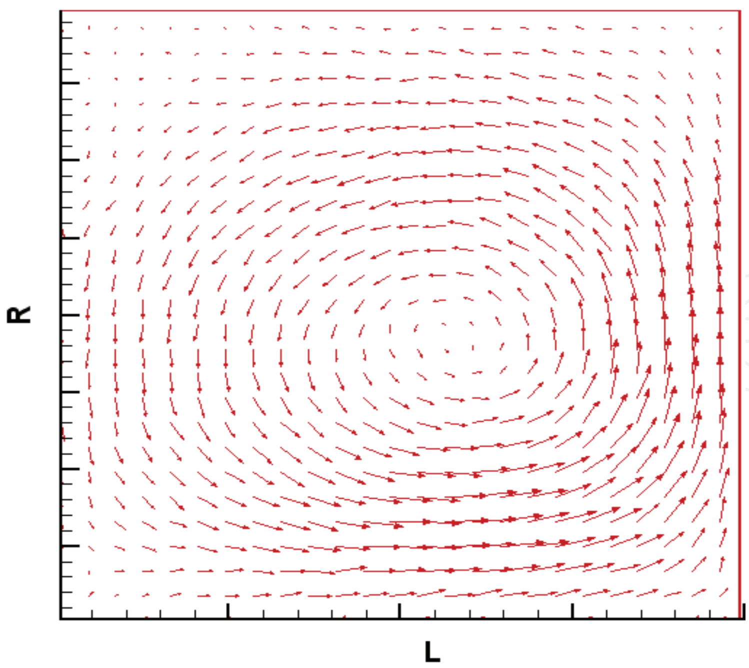

Fig. 8. Flow filed of single-vortex Flow $V_{\Theta 1} / (2R\,T_0)^{1/2} = 0.81$ $V_{\Theta 2} / (2R\,T_0)^{1/2} = -0.237$

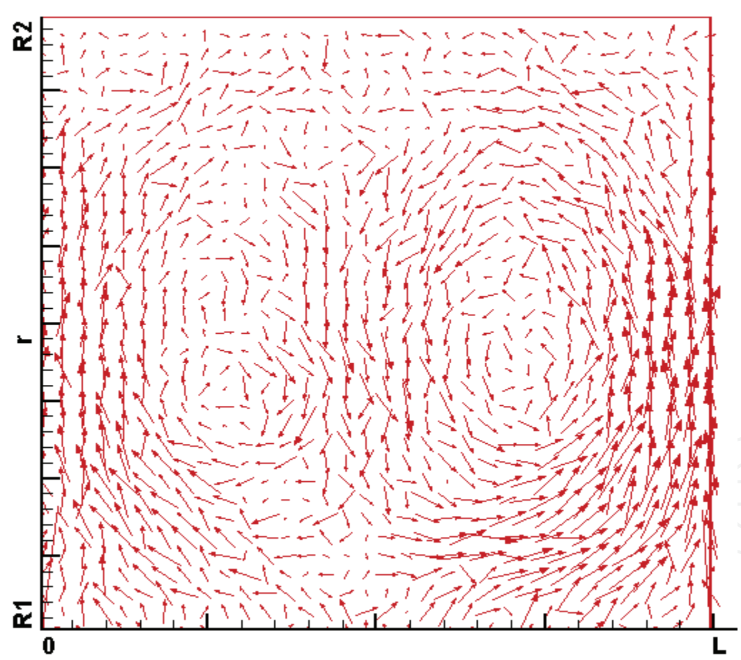

Fig. 9. Flow filed of double-vortex Flow $V_{\Theta 1} / (2R\,T_0)^{1/2} = 0.81$ $V_{\Theta 2} / (2R\,T_0)^{1/2} = -0.27$

Figure 8 shows the flow field of double-vortex flow at $V_{\Theta 1} / (2R\,T_0)^{1/2} = 0.81$ and $V_{\Theta 2} / (2R\,T_0)^{1/2} = -0.27$. Figure 10 Fig. 8 shows the flow field of single vortex flow at $V_{\Theta 1} / (2R\,T_0)^{1/2} = 0.81$ and $V_{\Theta 2} / (2R\,T_0)^{1/2} = -0.311$. It can be seen from these figures when pressure increases, we have weaker vortex flow. Figure 11 shows density when $V_{\Theta 1} = 1000$ m/s is constant and $V_{\Theta 2}$ is 200, 500 and 1000 m/s. According to this figure, if the velocity of the outlet cylinder increases, density changes rapidly. Figure 12 shows temperature changes when $V_{\Theta 1}$ = 1000 m/s is constant and $V_{\Theta 2}$ is 200, 500 and 1000 m/s. It can be seen that maximum temperature occurs when the velocity of the outlet cylinder is 200 m/s. Figure 13 shows radial velocity at 4, 40 and 400 Pa. The results show different flow patterns at different temperature and pressure.

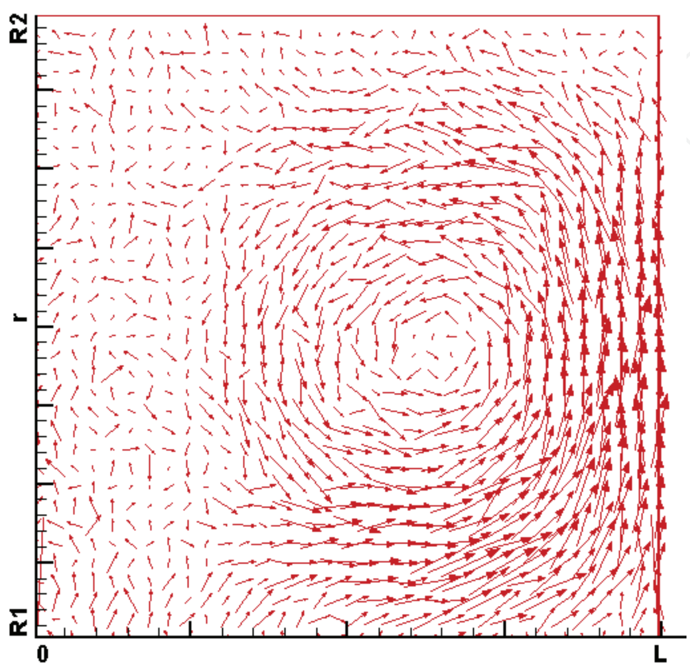

Fig. 10. Flow filed of single-vortex Flow $V_{\Theta 1} / (2R\,T_0)^{1/2}$ = 0.81 $V_{\Theta 2} / (2R\,T_0)^{1/2}$ =-0.311

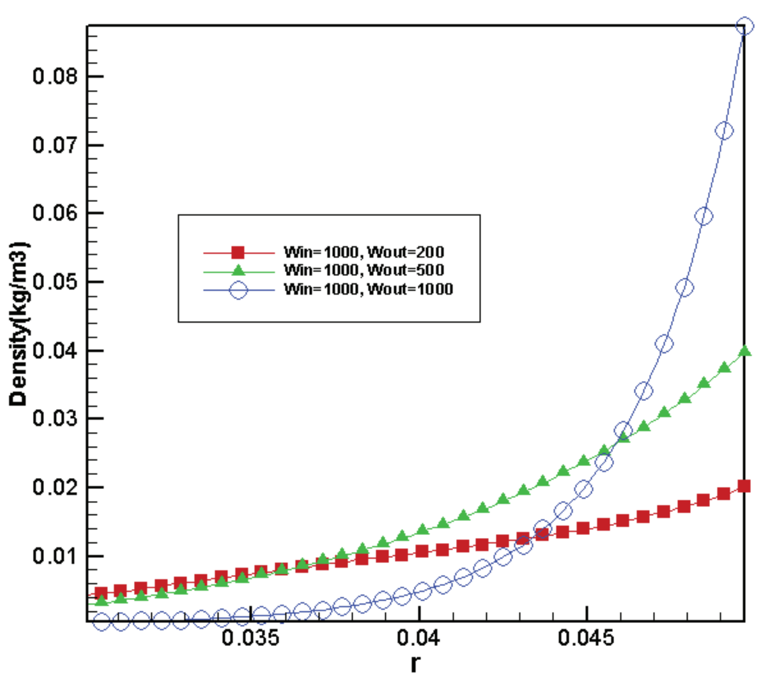

Fig. 11. Density at $V_{\Theta 1}$ = 1000 m/s is constant and $V_{\Theta 2}$ is 200, 500 and 1000 m/s

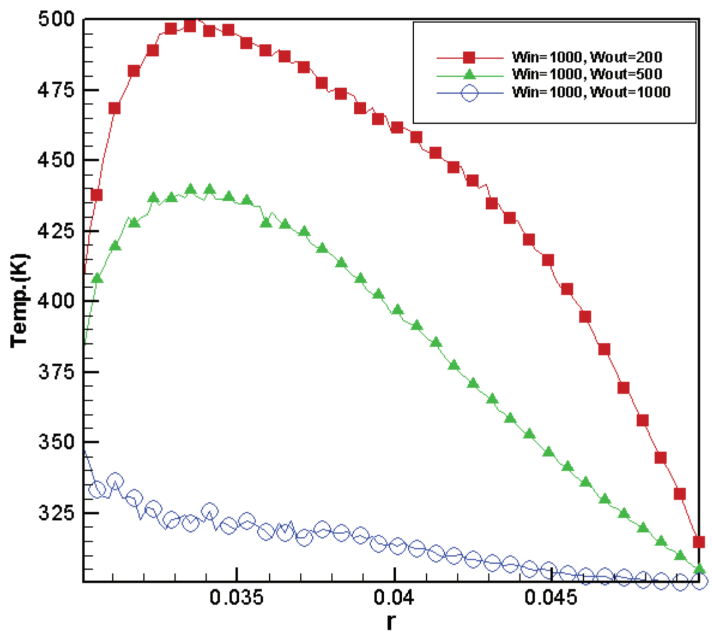

Fig. 12. Temperature changes at $V_{\Theta 1}$ = 1000 m/s is constant and $V_{\Theta 2}$ is 200, 500 and 1000 m/s.

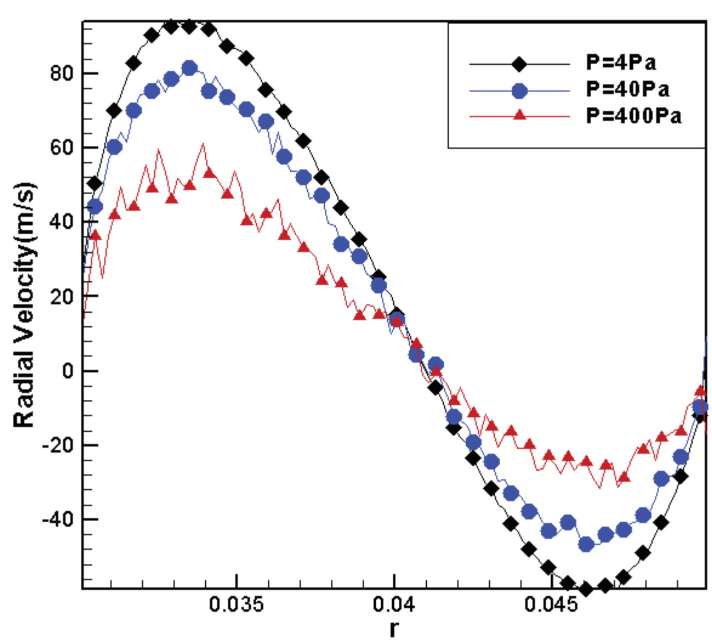

Fig. 13. Radial velocity at 4, 40 and 400 Pa

4. Conclusions

In this work, The Couette-Taylor flow for a rarefied gas is supposed to be contained in an annular domain, bounded by two coaxial rotating circular cylinders. The Boltzmann equation was solved with DSMC method. The results showed different type of flow patterns, as Couette-Taylor flow or single and double vortex flow, can be created in a wide range of speed of rotation of inner and outer cylinders. This work shows if size or number of cells is not proper, we cannot obtain reasonable results by using DSMC method.

5. Nomenclature

f = density distribution function
F = external forces filed
K = Boltzmann constant
K_n =Knudsen number
m = molecular wieght
p = pressure
Q = collision integral
T = temperature
$R1$ =radius of the inlet cylinder
$R2$ =radius of the outlet cylinder
T_{tr} =translational temperature
u = free stream velocity
v = molecular velocity
κ = molecular constant
μ = collision rate per unit of time and volume
ρ = density of gas
σ = hard sphere diameter
Subscripts
* = other investigated features
Superscripts
2 = two dimentional phase
3 = three dimentional phase
′ = value of feature after collision Abbreviations
DSMC = Direct Simulation Monte Carlo

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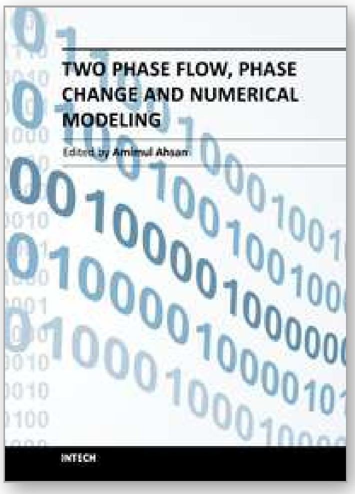

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The heat transfer and analysis on laser beam, evaporator coils, shell-and-tube condenser, two phase flow, nanofluids, complex fluids, and on phase change are significant issues in a design of wide range of industrial processes and devices. This book includes 25 advanced and revised contributions, and it covers mainly (1) numerical modeling of heat transfer, (2) two phase flow, (3) nanofluids, and (4) phase change. The first section introduces numerical modeling of heat transfer on particles in binary gas-solid fluidization bed, solidification phenomena, thermal approaches to laser damage, and temperature and velocity distribution. The second section covers density wave instability phenomena, gas and spray-water quenching, spray cooling, wettability effect, liquid film thickness, and thermosyphon loop. The third section includes nanofluids for heat transfer, nanofluids in minichannels, potential and engineering strategies on nanofluids, and heat transfer at nanoscale. The forth section presents time-dependent melting and deformation processes of phase change material (PCM), thermal energy storage tanks using PCM, phase change in deep CO2 injector, and thermal storage device of solar hot water system. The advanced idea and information described here will be fruitful for the readers to find a sustainable solution in an industrialized society.

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