

DSMC Simulation of Rarefied Gas Flow in a Single-sided and Double-sided Lid-Driven Cavity

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Abstract

The present study is to investigate the behaviour of a monoatomic gas enclosed in a cavity with both the top and bottom walls imparting motion to the fluid. The problem is studied for single and double-sided lid-driven flow for various wall velocities as well as parallel and anti-parallel wall motions. These types of flow have many industrial applications such as drying and melt spinning. In contrast to the single-sided flows the vortex patterns obtained in the double-sided flows are different and hence it merits a thorough examination, which is studied in this paper using the Direct Simulation Monte Carlo (DSMC) method. The DSMC method proposed by G.A. Bird is based on the kinetic theory in which the molecular motion is modelled stochastically. The computational model has been implemented in OpenFOAM software using the solver named dsmcFoam. Various flow features have been examined such as eddies and vortices.

Keywords: *Rarefied gas flows, DSMC, Knudsen number, Lid Driven cavity, Kinetic theory, Discrete methods.*

I. INTRODUCTION

The continuum assumption is not valid when the density of the fluid is very low or when the characteristic dimension of the problem is small, and the Navier Stokes equation cannot be applied to model the flow. Knudsen number ($Kn = \lambda/L$), the ratio of the mean free path to the characteristic dimension of the system under consideration, quantifies this. The range of the various regimes based on Kn and the suitable numerical technique applicable for each regime is given in Table 1. When the Knudsen number is high, there are errors of very high magnitude when the Navier Stokes equation are used to solve the flow problem; therefore we have to resort to other methods.

The Direct Simulation Monte Carlo (DSMC) method, formulated by G.A. Bird in 1960, is one such method which can be used to model the rarefied gas flows [1]. The DSMC method is based on the kinetic theory of gases. In DSMC the Boltzmann equation is stochastically solved to obtain a stable equilibrium flow field of molecules. The DSMC method is very reliable when it

comes to predicting the flow and heat transfer properties in all the flow regimes and is one of the widely used numerical methods.

Table.1. Kn number regimes, adapted from Ref. [2].

Kn Range	Type of Flow	Suitable Numerical Approach
$Kn \rightarrow 0$	Inviscid flow	Euler fluid equations
$Kn \leq 0.001$	Continuum regime	Navier–Stokes–Fourier fluid equations
$0.001 \leq Kn \leq 0.1$	Slip regime	Navier–Stokes–Fourier fluid equations with modified boundary conditions
$0.1 \leq Kn \leq 10$	Transition regime	Boltzmann equation or DSMC
$Kn \geq 10$	Free-molecular regime	Boltzmann equation or DSMC

Lid-driven cavity problem is one of the classic problems to understand the elementary flow features. In the present paper, the top and the bottom walls move and impart a motion to the fluid. The problem attempted has many industrial applications in the field of melt spinning, drying technologies and surface coating [3]. The cavity problem is also one of the most frequently explored problems from the academic viewpoint. During the last few decades, the cavity problem has been explored both experimentally and computationally [4]. Conventional numerical approaches such as Finite element, Finite volume and Finite difference are used to model the single-sided lid-driven problem [5]. Another typical instance is the case where both the walls move with uniform velocity and impart motion to the fluid. If the two walls move in the same direction, the flow is said to have a parallel motion, and if the two walls move in opposite direction, the flow is said to have anti-parallel motion. Many researchers have studied the double-sided lid-driven cavity problem using different numerical methods [6], [7]. Bhopalam et al. have recently studied double-sided cavity problem [8] using the Lattice Boltzmann method. Although various authors have

investigated the single-sided cavity problem for continuum flows, the same has not been done for rarefied gas flows, and the literature relating to the double-sided lid-driven cavity flow appears to be very scarce.

In this paper, the single and double-sided lid-driven cavity flow problem is studied for a monatomic gas Argon for different wall velocities and both parallel and antiparallel motions of the wall. An open source C++ code based solver known as dsmcFoam, based on the framework of OpenFOAM is used for computational modelling and simulation. The results obtained show the emergence of corner eddies as counter-rotating vortices on varying the aspect ratio, lid velocities and the direction of wall motion.

II. METHODOLOGY

A. Numerical methodology

In the present paper, the DSMC method is used. A detailed procedure of the DSMC method can be found in Bird [1]. The DSMC method is based on the Boltzmann's Equation with certain restrictions [9].

$$\frac{\partial n f}{\partial t} + c \cdot \frac{\partial n f}{\partial r} + F \cdot \frac{\partial n f}{\partial c} = \int_{-\infty}^{+\infty} \int_0^{4\pi} n^2 (f^* f_1^* - f f^1) c_r \sigma d\Omega dc_1$$

The above equation is an integro-differential equation in $n f$. Where n is the number density and f is velocity distribution function. c represents the molecular velocity, r the relative molecular speed and F is an external force. The superscript * indicates post-collision values, f and f^1 represent two different types of molecules, σ is the collision cross-section, and Ω is the solid angle.

The reference pressure P at which the simulations are carried out is given by $P = nkT$ and the mean free path is defined by the equation,

$$\lambda = \frac{\mu}{P} \sqrt{\frac{\pi RT}{2}}$$

In the DSMC algorithm, the flow field is divided into various cells in which the sampling of the microscopic properties takes place. Collisions are permitted within the same cell or sub-cell. Collision model and molecular interaction used are a Variable hard sphere (VHS) and Larsen-Borgnakke (LB) collision model, respectively. The No Time Counter (NTC) scheme is chosen to model the collision pairs. In this work, the solid walls are modelled using the diffuse reflection model with full thermal accommodation coefficient. For all the calculations the monoatomic gas argon is used with mass $m=6.63 \times 10^{-26}$ kg and with a reference particle diameter of $d=4.17 \times 10^{-10}$ m. As per the general guidelines of the DSMC method, the cell size is smaller than the mean free path and the time step is less than the mean collision time respectively. To minimise the statistical noise in the sampling of flow variables, 25 Particles per cell (PPC) are considered.

B. Geometry of the problem

The geometry considered for simulation is given in Figures 1,2 and 3. In the first case, only the top wall is moving, and the other walls are fixed, whereas in the second case both the top and bottom walls are moving either in parallel or antiparallel direction. L represents the length and height of the square cavity. The points A, B, C, D represent the four corners of the cavity. The length and height of the domain are 1m, and the flow is neglected in the z -direction making it a 2D problem. The flow is simulated for different wall velocities U_w such as 10,50,100 and 200 m/s. All the walls are maintained at a constant temperature of 273K respectively.

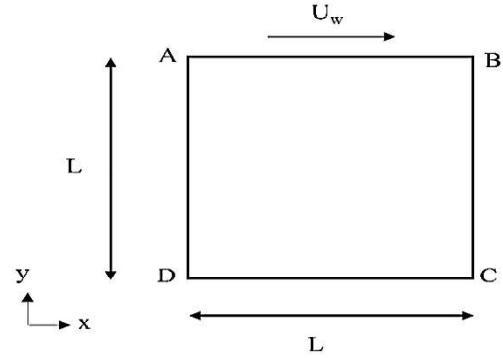


Figure 1. Single-sided cavity with a moving top wall.

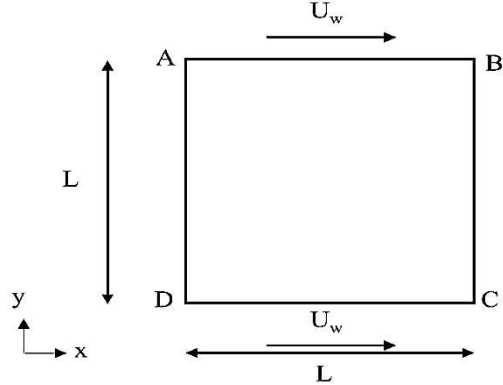


Figure 2. Double-sided cavity with parallel wall motion

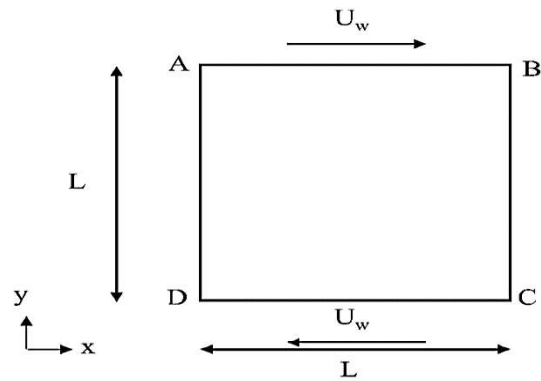


Figure 3. Double-sided cavity with anti-parallel wall motion.

C. Mesh details

The flow domain is equally divided into 100x100 cells in the x and y directions to capture the physics of the problem accurately. Grid independence test was carried out for three different meshes coarse, medium and fine i.e. 75x75, 100x100 and 125x125. Figure 5 shows the vertical velocity profile along the horizontal centreline. The variation in results for the medium and fine grid was not significant. Hence a grid size of 100x100 was used for the rest of the study. The timestep Δt was 2×10^{-6} which was much smaller than the mean collision time. The number of simulated particles was around 5 lakhs. The meshed domain is as shown in Figure 4.

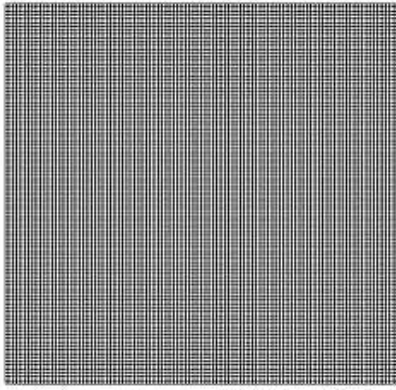


Figure 4. The meshed domain of 100x100 cells.

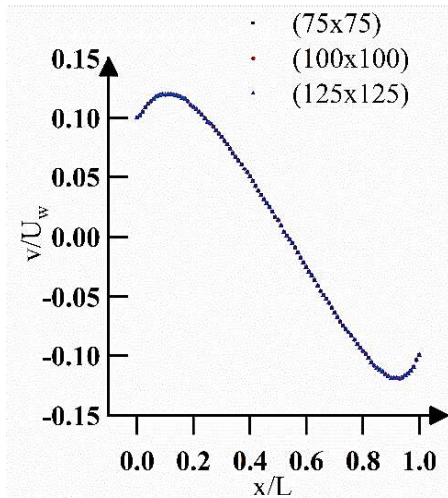


Figure 5. Vertical velocity distribution on the horizontal centerline for different grids.

D. Free stream conditions

The free stream conditions considered for the present simulation are given in the Table 2.

Table.2. Free stream conditions.

T_{∞} (K)	p_{∞} (N/m ²)	ρ_{∞} (kg/m ³)	μ_{∞} (Ns/m ²)	λ_{∞} (m)
273	0.007	1.23×10^{-7}	2.1×10^{-5}	0.896

Referring to Table 2, T_{∞} , p_{∞} , ρ_{∞} , μ_{∞} , λ_{∞} , refer respectively to the temperature, pressure, density, viscosity, and mean free path.

E. Validation of the problem

The validation study of the dsmcFoam solver is performed by comparing the results obtained by the present study with that of a similar problem studied by John et al. [10] and the comparative plots are plotted in Figure 6. Results are plotted for the u velocity profile along vertical line at the centre of the cavity. The close agreement between the results can be observed which validates the study.

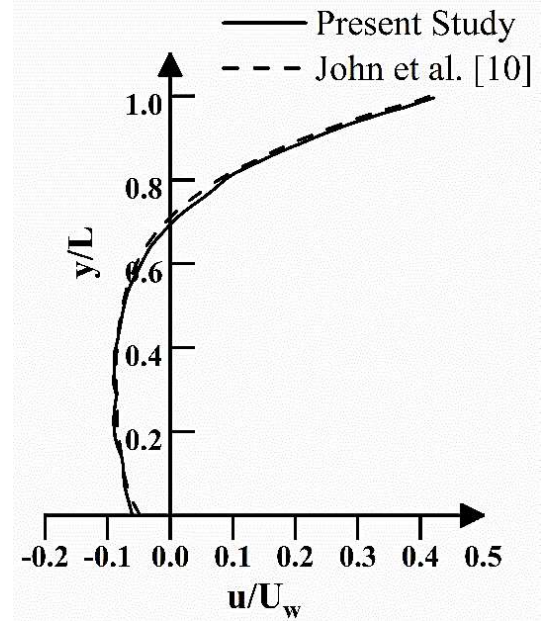


Figure 6. Comparison of results with Reference [10].

III. RESULTS AND DISCUSSION

In order to predict flow features in the cavity, four different lid velocities, i.e., $U_w = 10, 50, 100, 200$ m/s were considered. The Mach numbers corresponding to the above lid velocities were 0.032, 0.16, 0.32 and 0.64 and the Reynolds numbers were 1, 5, 10 and 20 respectively. The Kn for all the cases was fixed to close to 1.

The velocity streamlines superimposed on the pressure contours for the single-sided, and the double-sided lid-driven cavity is as shown below. Figure 7 is for single-sided case where the top wall is moving at 200 m/s. Figures 8 and 9 are for the double-side case where the top and bottom walls are moving at 200 m/s in the parallel and anti-parallel directions respectively. From Figure 9, we see that the vortices in antiparallel wall motion case are symmetric with respect to the vertical centreline. This is unlike the other two cases, owing to symmetry in the boundary conditions.

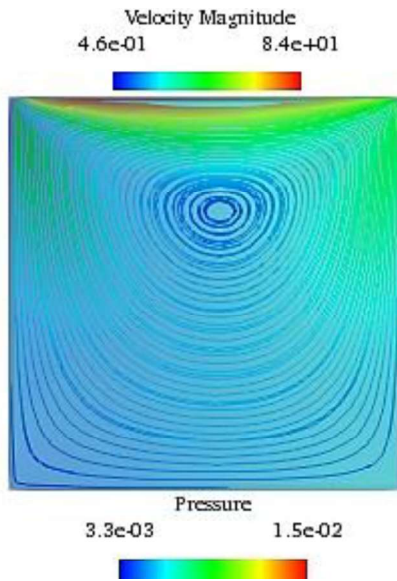


Figure 7. Velocity streamlines overlaid on pressure for $U_w = 200$ m/s.

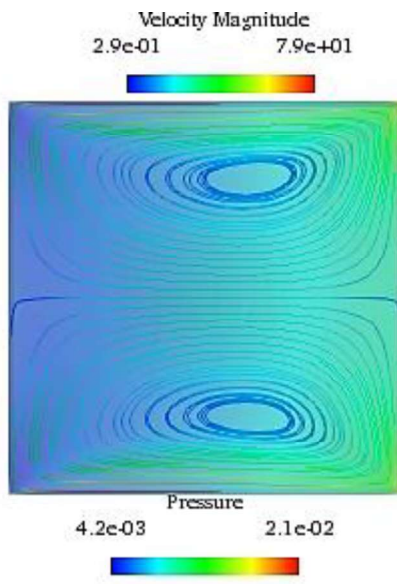


Figure 8. Velocity streamlines overlaid on pressure for $U_w = 200$ m/s for anti-parallel wall motion.

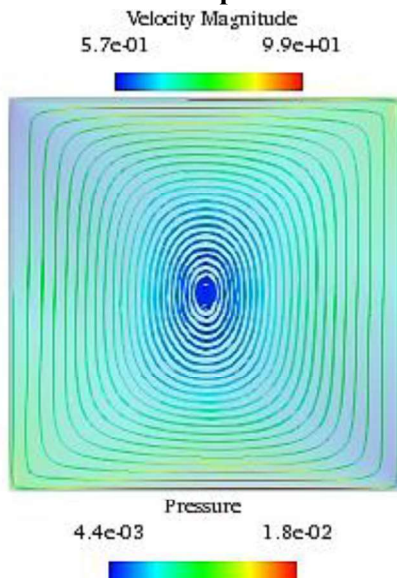


Figure 9. Velocity streamlines overlaid on pressure for $U_w = 200$ m/s for parallel wall motion.

IV. CONCLUSIONS

In this study, the DSMC method is used to study the single and double-sided lid-driven cavity using the `dsmcFoam` solver. The flow patterns for different wall motion has been investigated. The `dsmcFoam` solver is validated by comparison with well-established results from the literature. The significant results include the position of vortex centres and their corresponding sizes. Results show two primary counter-rotating vortices for the parallel wall motion whereas only one primary vortex for anti-parallel wall motion. Our results show that the DSMC method can capture the flow features in the transitional regime reasonably well. Further work needs to be carried out to explore the other flow regimes.

REFERENCES

- [1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford, New York: Oxford University Press, 1994.
- [2] M. Gad-el-Hak, "The Fluid Mechanics of Microdevices—The Freeman Scholar Lecture," *J. Fluids Eng*, vol. 121, no. 1, pp. 5–33, Mar. 1999.
- [3] M. M. Gupta and J. C. Kalita, "A new paradigm for solving Navier–Stokes equations: stream function–velocity formulation," *Journal of Computational Physics*, vol. 207, no. 1, pp. 52–68, Jul. 2005.
- [4] A. B. Cortes and J. D. Miller, "Numerical experiments with the lid driven cavity flow problem," *Computers & Fluids*, vol. 23, no. 8, pp. 1005–1027, Nov. 1994.
- [5] M. Cheng and K. C. Hung, "Vortex structure of steady flow in a rectangular cavity," *Computers & Fluids*, vol. 35, no. 10, pp. 1046–1062, Dec. 2006.
- [6] H. C. Kuhlmann, M. Wanschura, and H. J. Rath, "Flow in two-sided lid-driven cavities: non-uniqueness, instabilities, and cellular structures," *Journal of Fluid Mechanics*, vol. 336, pp. 267–299, Apr. 1997.
- [7] D. Arumuga Perumal and A. K. Dass, "Multiplicity of steady solutions in two-dimensional lid-driven cavity flows by Lattice Boltzmann Method," *Computers & Mathematics with Applications*, vol. 61, no. 12, pp. 3711–3721, Jun. 2011.
- [8] S. B. R., D. A. Perumal, and A. K. Yadav, "Computation of fluid flow in double sided cross-shaped lid-driven cavities using Lattice Boltzmann method," *European Journal of Mechanics - B/Fluids*, vol. 70, pp. 46–72, Jul. 2018.
- [9] C. Cercignani, *The Boltzmann Equation and Its Applications*. New York: Springer-Verlag, 1988.
- [10] B. John, X.-J. Gu, and D. R. Emerson, "Investigation of Heat and Mass Transfer in a Lid-Driven Cavity Under Nonequilibrium Flow Conditions," *Numerical Heat Transfer, Part B: Fundamentals*, vol. 58, no. 5, pp. 287–303, Nov. 2010.