Monte Carlo Simulation of Rotation of A Laser Opto-Microactuator

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Abstract. The rotation of a laser opto-microactuator with a four blades rotor system immersed in a low density gas is analyzed by using DSMC method. The range of the Knudsen number (based on the blade size) Kn=01 – 0.2 was chosen close to the experimentally established values for which the rotation rate reached maximum. A new computational prediction-correction procedure is proposed for DSMC calculation of gas flows with widely separated kinetic relaxation and macroscopic evolution time scales. In case of a rotating micro-mechanical system the procedure allows significant reduction of the computational time needed to approach the established regime of rotation.

Keywords: rotating MEMS, rarefied gas, DSMC.
PACS: 47.61.Fg, 47.45.-n, 47.32.-y, 52.65.Pp

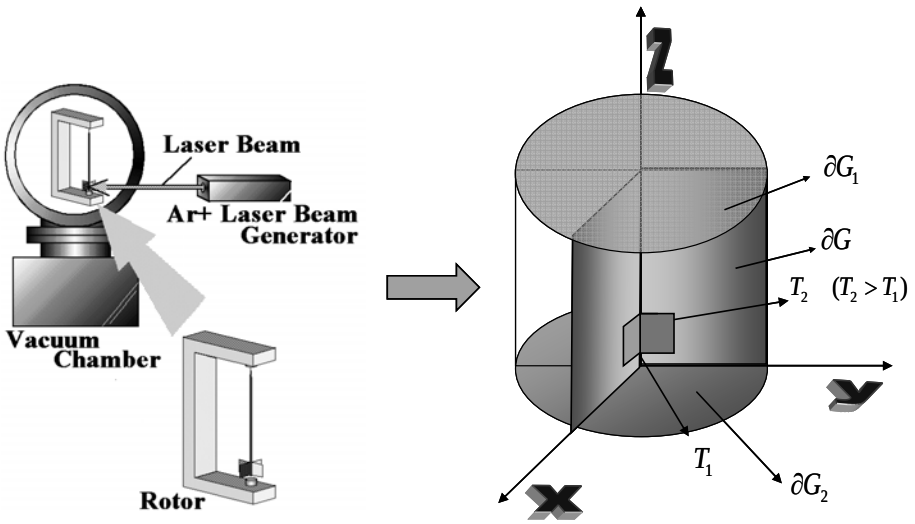
INTRODUCTION

The rapidly developing micro and nano technologies suggests new challenges for investigation of original microsized mechanical system working in a medium that no longer can be treated as continuum. Moreover, the relevant experimental work should be supported by a subtle theoretical and computational analysis taking into account the non-equilibrium and non-continuum effects in the micro system. In the present paper we demonstrate this approach by a DSMC analysis of the rotation of a laser opto-microactuator with a four blades rotor system immersed in a low density gas [1]. The rotor system is rotated by a driving force of rarefied dynamic effects arising around each blade due to the temperature difference between front and rear blade sides created and held by remote laser heating. To simulate of a rotating configuration the standard DSMC method [2] must be modified significantly. The simulation is carry out in a rotating coordinate system fixed to the blade system. Thus the particle motion and the boundary conditions are to be transformed with respect to the rotating coordinate system. The basic computational difficulty of the DSMC simulation of the rotation system is not the large number of coordinate and velocity transformations but the fact that the kinetic time scale of the gas flow around the blade system is widely separated from the macroscopic time scale of the blade rotation – the mean collision time is about 10^{-6} s while the rotor reaches an established rotation rate for about 10-20 s. This difficulty was overcome by using a new prediction-correction procedure that allowed the computational time to be shortened more than ten times. The proposed prediction-correction procedure can be used as a universal tool together with the standard DSMC method for simulation of gas flows with widely separated kinetic relaxation and macroscopic evolution time scales

Three-dimensional DSMC calculations were performed for Knudsen numbers (based on the blade size) Kn=01 – 0.2 that were close to the experimentally established values for which the rotation rate reached maximum [1]. The temperature difference between the blade front and rear surfaces was 15K. In general, the obtained numerical results for the rotation rate agree with the experimental data qualitatively. The growth of the calculated rotation rate within the transient period corresponds to the experimental observations but the established value overpredicts more than twice the obtained from the experiment. In our opinion, one of the underlying reasons for the discrepancy might be linked with the temperature difference between front and rare sides of the rotor blades which is kept constant in the simulation while the experiment shows that it pulsates in accordance with the blade system rotation. This problem will be investigated in a subsequent study.

COMPUTATIONAL MODEL OF THE ROTATING BLADE SYSTEM

A schematic drawing of the laser opto-microactuator is shown in Fig.1 (a). The rotor four blade system is kept fixed via a needle shaft and a system of two magnets which has a very small friction. Each blade is one-side coated with carbon black powder to absorb better the laser beam energy. The laser is situated outside the vacuum chamber filled with a low density gas as shown in Fig. 1 (a). In result of the laser irradiation the coated side of each blade is heated to temperature T_2 larger than the temperature T_1 of the rear side of the blade. The temperature difference makes the total kinetic moment of all gas molecules hitting the blades on both sides different from zero and the blade system starts rotating. An established rotation rate is reached when the kinetic moment is equalized to the total resistance momentum exerted by the rotor



(a) (b)

FIGURE 1. Schematic drawings of the opto-microactuator (a) and the corresponding three-dimensional computational model of the rotor blade system (b).

Taking into account the existing symmetries of the rotor system the DSMC calculations have been carried out in a three-dimensional computational domain occupying the first octant of a Cartesian coordinate system (Fig 1 (b)) that rotates in conjunction with the blade system around the z-coordinate fixed to the rotor axis. Initially, the domain is filled with gas with density n_0 and temperature T_0 in equilibrium with the chamber walls. The circumferential velocity $\mathbf{V}_\tau(t)$ of the coordinate system is related to the angular velocity $\omega(t)$ of rotation as follows

$$\mathbf{V}_\tau(t) = \omega(t) r \boldsymbol{\tau}, \tag{1}$$

where $r = \sqrt{x^2 + y^2}$ and $\boldsymbol{\tau}$ is tangential unit vector. Open boundary conditions are imposed at the side and top boundaries ∂G and ∂G_1 of the computational domain,

$$\partial G = \left\{(x, y) \in x^2 + y^2 = R^2, z \in (0, H)\right\}, \tag{2}$$

$$\partial G_1 = \left\{(x, y) \in x^2 + y^2 < R^2, z = H\right\}. \tag{3}$$

Within each time step of the simulation all particles going out through these boundaries are removed from further consideration and a number of new particles enter in according with the velocity distribution

$$f(t,\mathbf{x},\boldsymbol{\xi}) = \frac{n_0\beta^3}{\pi^{3/2}}\exp\left[-\beta^2\left(\boldsymbol{\xi}-\mathbf{V}_\tau\right)^2\right], \quad (\boldsymbol{\xi}.\mathbf{n}) < 0, \tag{4}$$

where $\beta = 1/2RT_0$, $\mathbf{x} = (x, y, z)$, $\boldsymbol{\xi} = (\xi_x, \xi_y, \xi_z)$ and $\mathbf{n}$ are particle velocity and unit vector normal to the boundary. At the bottom boundary ∂G_2.

$$\partial G_2 = \left\{(x, y, z) \in x^2 + y^2 < R^2, z = 0\right\} \tag{5}$$

all particles are reflected diffusively according to the velocity distribution

$$f(t,\mathbf{x},\boldsymbol{\xi}) = \frac{n_w\beta^3}{\pi^{3/2}}\exp\left[-\beta^2\left(\boldsymbol{\xi}-\mathbf{V}_\tau\right)^2\right], \quad (\boldsymbol{\xi}.\mathbf{n}) > 0, \tag{6}$$

where n_w is number density of the reflected particles. At the coordinate planes Oxz and Oyz we impose a condition of periodicity that is a particle going out through one of both coordinate planes enters through the other with a corresponding velocity. Each particle hitting a blade surface is reflected diffusively with velocity corresponding to temperature T_1 on the blade surface at Oxz and T_2 on the blade surface at Oyz $(T_2 > T_1)$.

Dynamic Equation of The Rotating Blade System

The dynamic equation of the rotating system of four blades can be reduced to an equation for one blade in the considered computational domain. Here we neglect the presence of the holding needle shaft. The momentum equation can be written in the following differential form

$$J_{blade}\frac{d\omega(t)}{dt} = M_{xz}(t) - M_{yz}(t), \tag{7}$$

$$M_{xz}(t) = \lim_{\Delta\tau\to 0}\left\{\frac{m}{\Delta\tau}\left[\left(\sum_{i=1}^{N_i} r_i(t)\left(\boldsymbol{\xi}_i(t)\cdot\mathbf{n}\right)\right)_{\boldsymbol{\xi}_i\cdot\mathbf{n}>0} + \left(\sum_{i=1}^{N_i} r_i(t)\left(\boldsymbol{\xi}_i(t)\cdot\mathbf{n}\right)\right)_{\boldsymbol{\xi}_i\cdot\mathbf{n}<0}\right]\right\} \tag{8}$$

$$M_{yz}(t) = \lim_{\Delta\tau\to 0}\left\{\frac{m}{\Delta\tau}\left[\left(\sum_{j=1}^{N_j} r_j(t)\left(\boldsymbol{\xi}_j(t)\cdot\mathbf{n}\right)\right)_{\boldsymbol{\xi}_j\cdot\mathbf{n}>0} + \left(\sum_{j=1}^{N_j} r_j(t)\left(\boldsymbol{\xi}_j(t)\cdot\mathbf{n}\right)\right)_{\boldsymbol{\xi}_j\cdot\mathbf{n}<0}\right]\right\}, \tag{9}$$

where $\boldsymbol{\omega}(t) = \{0, 0, \omega(t)\}$ is the angular velocity of rotation. The axis of rotation coincides with axis Z. $M_{xz}(t)$ and $M_{yz}(t)$ are the total kinetic momentums of the all incident and reflected particles within time $\Delta\tau$ on the corresponding sides of the blade; $J_{blade} = (\rho ab/3)c$ is the inertial moment of the blade, a, b is the blade size in x (or y) and z direction, respectively, c is the blade thickness. The time interval of particle momentum collection $\Delta\tau$ is very small regarding to the macroscopic scale of the rotation. The choice of the time intervals will be discussed in the following paragraph.

Time Prediction-Correction Algorithm

The time scales of the kinetic gas relaxation and the macroscopic scale of rotation of the blade system are widely separated. That is why, a straightforward application of the standard DSMC algorithm is not effective and the computational procedure must be modified. To this aim we consider three levels of time consideration: the first is kinetic relaxation time within which the standard DSMC method is applied to advance the simulation with a time step Δt. The second time level is linked to macroscopic data collection within time interval $\Delta\tau = K\Delta t$, which is small compared to the third time level of macroscopic consideration of the rotation of the blade system. However, the time $\Delta\tau$ is large enough regarding to the kinetic relaxation scale for collecting a meaningful sample size. In our consideration the number of kinetic steps passed for collection of a macroscopic data set is $K = 200$ that was

sufficient for our aim. On the third level we assume that the time evolution of the rotation can be approximate by a linear function within a time interval $\Delta T = M\Delta\tau$. Thus we have the following order of the time intervals used in the prediction-correction procedure $\Delta T >> \Delta\tau >> \Delta t$ before to compute a prediction value of the rotation rate over a large time interval . Taking into account these assumptions as well as the rotation of the coordinate system the basic steps of the DSMC procedure are as follows:

- the standard DSMC algorithm is used to move and collide particles within each kinetic step Δt neglecting the rotation of the coordinate system. For Δt the change of the axis positions can be neglected. In a stationary frame the new position of each particle is given by

$$x'(t+\Delta t) = x'(t) + \xi'(t)\Delta t\,. \tag{10}$$

In the rotation frame the new position of each particle is transformed as follows

$$x(t+\Delta t) = A(\omega\Delta t)x'(t+\Delta t)\,. \tag{11}$$

where the matrix of rotation has the form

$$A(\omega\Delta t) = \begin{pmatrix} \cos\omega\Delta t & \sin\omega\Delta t & 0 \\ -\sin\omega\Delta t & \cos\Delta\omega t & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{12}$$

The particle velocity vector is also updated in accordance with the formula [3]

$$\xi(t+\Delta t) = \xi'(t) - \omega\times x(t+\Delta t)\,. \tag{13}$$

For the next time step we accept that

$$x'(t) = x(t); \qquad \xi'(t) = \xi(t).. \tag{14}$$

To pass a step $\Delta\tau$ the described procedure (10) – (14) is repeated K times ($\Delta\tau = K\Delta t$) and the macroscopic data are collected for obtaining the rotation velocity growth $\Delta\omega(t)$ from equation (7).

The new velocity of rotation is equal to

$$\omega(t+\Delta\tau) = \omega(t) + \Delta\omega(t)\,. \tag{15}$$

The whole procedure described above is repeated M times to pass a large step ΔT needed for creating a prediction for the next value of the angular velocity when jumping over a large time interval. The steps described with equations (10)- (15) illustrate the correction stage of the prediction-correction procedure. The simplest way for elaborating a prediction value for the angular velocity of the rotor over a time interval T $(T >> \Delta T)$ is given by the formula

$$\omega(t+\Delta t) = \omega(t) + \frac{\omega(t+\Delta T) - \omega(t)}{\Delta T}T\,. \tag{16}$$

The final step of the prediction procedure is to update the velocities of all particles in accordance with the new velocity of rotation of the coordinate system

$$\xi(t+T) = \xi'(t+T) - \Delta\omega\times x'(t+T)\,. \tag{17}$$

Thus the prediction stage consists of two steps described with formulas (16) and (17). The set of coordinates $\mathbf{x}'(t+\mathrm{T})$ and velocities $\boldsymbol{\xi}'(t+T) = \boldsymbol{\xi}(t+T)$ of all particles in the computational domain is the new initial state for the next correction stage (10) - (15). The complete prediction-correction procedure is repeated in time until an established rotation rate is reached.

RESULTS

The approach described in the previous section is used to simulate by DSMC method the rotation of a microactuator that had been used in the experiment [1]. The computational domain is confined in a volume with radius $R = 0.03$ m and height $H = 0.03$ m. The blade size is 5×5 mm and the blade thickness is 0.1 mm. In our consideration the rotor system consists of four blades made from pyrex ($\rho = 2230$ kg/m^3) and we do not take into account the shaft holding it. The blade thickness is also neglected. Initially, the domain is assumed to be filled with air gas with number density $n_0 = 4\times10^{21}$ at temperature $T_0 = 288^o K$ that is equal to the ambient temperature.

Thus the pressure inside the vacuum chamber is about 8 Pa. The irradiated by laser beam front side of each blade is assumed to keep an averaged temperature $T_2 = 315^o K$, and respectively, the rear side - $T_1 = 300^o K$.

The Knudsen number based on the blade size is equal to $Kn = 0.13$ that is in the range of Knudsen numbers where a maximum rotating rate was obtained in the experiment. The time evolution of the rotation rate measured in the experiment [1] is shown in Fig.2

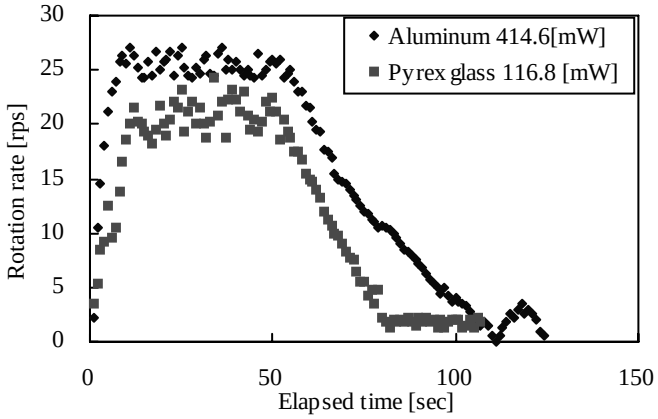


FIGURE 2. The rotation rate obtained from the experiment

The DSMC calculations are carried out for hard sphere molecules. The time steps used in the prediction-correction procedure are $\Delta t = 1.0 \times 10^{-6}$ s, $\Delta \tau = 200 \Delta t = 2.0 \times 10^{-4}$, $\Delta T = 2.0 \times 10^{-2}$ s, and the time interval of prediction is $T = 1.0$ s. The obtained results for the rotation rate are shown in Fig. 3. The graphic presents the time evolution of the rotation rate over the whole transient period. One can easy calculate that if the standard DSMC is used with time step $\Delta t = 1.0 \times 10^{-6}$ a more than 1.0×10^8 steps will be needed to approach the established regime of rotation. As seen from Figures 2 and 3 the growth of the calculated rotation rate within the transient period corresponds to the experimental observations but the established value overpredicts more than twice the obtained from the experiment.

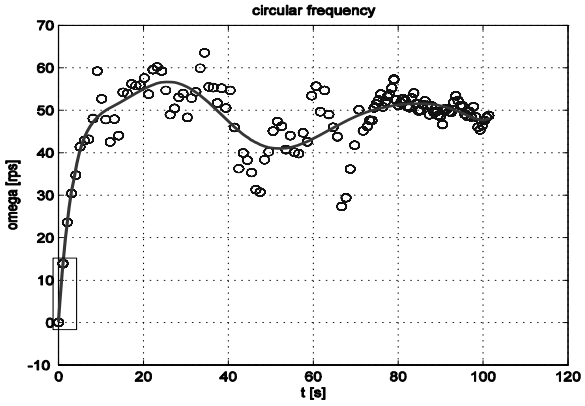


FIGURE 3. The rotation rate obtained from the DSMC calculations. The DSMC results are seen as circles representing the rotation rate within each time step of the prediction-correction procedure. The solid line represents the fitted results.

There are two underlying reasons for the difference detected between calculated and experimental results. The first is that in the DSMC analysis we have simplified the rotor configuration neglecting the presence of the holding shaft. The second is linked with the temperature difference between front and rare sides of the rotor blades which is kept constant in the simulation while the experiment shows that temperature pulsates simultaneously with the blade system rotation. Thus the effective temperature difference might be less than the accepted in the calculation. These problems are subject of our future investigations.

If we zoom the rectangle shown in Fig. 3 one can see that the enclosed first two markers are actually spots of circles representing the results of the first two time step of the prediction correction procedure. This is clearly seen in Fig. 4 (upper graphic). If we zoom now the rectangle in Fig. 4 (with the second spot enclosed) we obtain the actual distribution of the results obtained over a step ΔT of the prediction-correction procedure shown in Fig 4 (lower graphic). Thus Figures 3 and 4 illustrate the action of the proposed prediction-correction procedure.

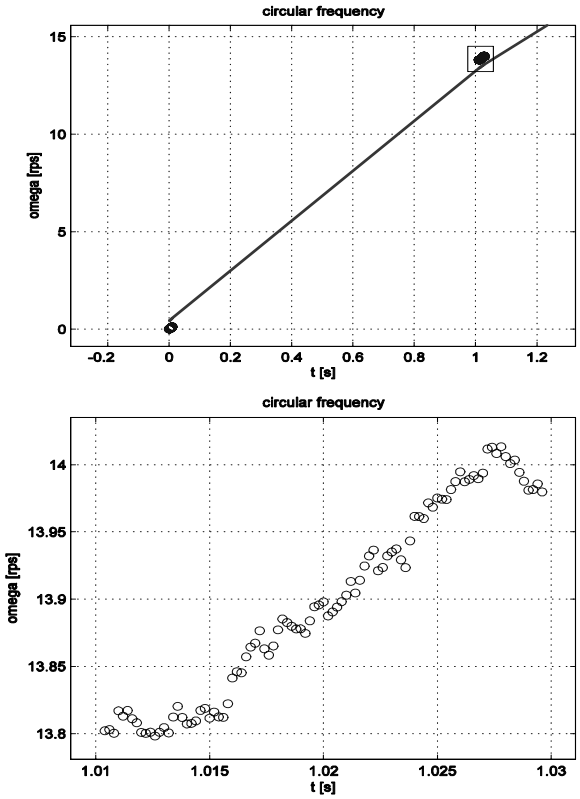


FIGURE 4. The zoomed rectangular window from Fig. 3 is presented in the upper graphic. The lower graphic shows the actual distribution of the calculated rotation rates within a time period ΔT This set is used to elaborate the next prediction value for a jump over time interval T.

CONCLUSIONS

Three-dimensional DSMC calculations are performed to simulate the rotation of the opto-microactuator considered in [1]. The proposed prediction-correction procedure can be used as a universal tool together with the standard DSMC method for simulation of gas flows with widely separated kinetic relaxation and macroscopic evolution time scales

ACKNOWLEDGMENTS

The research described in this paper was supported partially by the Bulgarian Ministry of education and science with Grant MM 1404/2004 also Grant-in-aid for Scientific Research ,No.16560154, 2004, Japanese Ministry of Education, Science and Culture.

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