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Research Note

Development of micro gas actuator for analyzing gas mixture

H. Wu[a], R. Moradi[b], M. Barzegar Gerdroodbary[c], and M. Shahbazi[d,*]

a. *Hubei Key Laboratory of Power System Design and Test for Electrical Vehicle, Hubei University of Arits and Science, Xiangyang 441053, China.*
b. *Department of Chemical Engineering, School of Engineering & Applied Science, Khazar University, Baku, Azerbaijan.*
c. *Department of Mechanical Engineering, Babol University of Technology, Babol, Iran.*
d. *Department of Electrical Engineering, Faculty of Engineering, Bu-Ali Sina University, Hamedan, Iran.*

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Abstract. In this study, a computational technique is used to investigate the ability of a new Micro Electro-Mechanical System (MEMS) gas actuator Microscale In-plane Knudsen Radiometric Actuator (MIKRA) for detecting and sensing gas mixture. In this actuator, the temperature difference of two arms in a rectangular domain in a rarefied condition induces a Knudsen force which is associated with physical properties of the gas. Both 2D and 3D approaches were applied to simulating the flow inside the model. In order to define the flow feature of low-pressure gas inside the micro gas actuator, a high-order equation of Boltzmann should be solved to attain reliable results. Since the domain of this micro gas is non-equilibrium, Direct Simulation Monte Carlo (DSMC) method was applied to the simulation of the model. According to obtained results, the three-dimensional model achieved more reliable results and the existence of a gap for the three-dimensional model clearly demonstrated the impact of this parameter on the effective Knudsen force.

1. Introduction

Lately, the importance and application of gas actuators to various engineering and industrial devices have increased. Gas actuators are widely used for the measurement and detection of dangerous gases such as CO and Ammonia. In addition, the initial step for the separation of the mixture is the detection of components of the mixture. Therefore, the improvement of this actuator could highly improve the measurement techniques in the industrial and scientific applications [1–3]. Furthermore, numerous investigators have motivated to improve a new simple method for recognizing hazardous and harmful gas such as ammonia, carbon oxide, and hydrogen.

Since the current gas actuator is expansive and costly, researchers have remained motivated to find new systems and methods that are cost effective and efficient. The advances of Micro-Electro-Mechanical System (MEMS) have allowed investigators to reduce the size of instruments on a micro scale. Therefore, microactuators are vastly industrialized because of their solicitations for the diverse methods and applications such as biomedical and bioengineering devices. One of the approaches detecting gas species within mixtures is the use of Knudsen force. Actually, the non-uniformity of the temperature of the rarefied gas yields a force recognized as Knudsen force. Former researches [4,5] exhibited that this kind of force was extremely sensitive

*. *Corresponding author.*
E-mail address: m.shahbazi@basu.ac.ir (M. Shahbazi)

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to the main characteristics of the gas species. These superior properties have encouraged the investigators [6] to use this method for pressure evaluation.

An extraordinary number of scholarships and works have been dedicated to determining the properties of the Knudsen force in low-pressure conditions. In a very good review paper by Ketsdever et al. [7], complete literature surveys were presented to reveal the history and origin of the Knudsen force. Furthermore, the nature of the Knudsen force was clarified and analyzed in their article. Crookes radiometer [8] is recognized as the first device that applied Knudsen force, and several scientists performed a large number of works and investigations on this device. Passian et al. [9] examined the specific mechanism of thermal transpiration on a micro scale via a Crookes cantilever. Furthermore, they [10–16] investigated the effect of thermal differences on the Knudsen forces in the transitional regime.

Direct Simulation Monte Carlo (DSMC) is a conventional technique for simulating the flow within the low-pressure domain. Darbandi and Sabouri [17,18] studied the effect of diffusive mass transfer on the rarefied gas mixing simulations. Some researchers [19,20] applied this approach to the simulation of hypersonic flow and micro channel. Ebrahimi and Roohi [21] focused on DSMC examination of low-pressure gas flow through diverging micro- and nano-channels. Vo et al. [22] employed both experimental and numerical techniques for studying Knudsen force.

Lately, Strongrich et al. [23,24] presented a new microsensor (Figure 1(a)) according to the mechanism of Knudsen force. They created Microscale In-plane Knudsen Radiometric Actuator (MIKRA) that would work in case of temperature variations among the two arms in the rarefied condition. In this actuator, the hot arm is motionless, while the cold arm may change. Since the gap of these two arms is too small, the Knudsen force exerts force on the cold side and this could be measured by the capacitor. Numerical simulations showed that there were two other types of the mechanism, which induced force on the cold arm. Figure 1(b) schematically presents the main mechanisms inside the MIKRA. The description of each type of flows will be comprehensively presented in the next chapters.

Although numerous scholars have investigated the radiometric force, most of research works have focused on the vane radiometer wherein hot and cold sides are the two sides of the vane. In fact, the features of Knudsen thermal force are not appropriately considered as hot and cold elements that exist in front of each other. In our previous works [25–34], the effect of Knudsen thermal force on the main characteristics of the rarefied MEMS actuator has been completely investigated. However, the performance of MIKRA has not been investigated experimentally or numerically for gas mixtures such as helium and methane with distinct chemical properties. In fact, the effects of mass concentration of each component have not been revealed. Therefore, the study of the flow feature and the main mechanisms of force generation inside the MIKRA in different conditions is essential for the development of the device. It should be mentioned that the numerical approach is widely applied to the simulation of industrial problems [35–53].

In the present paper, a computational technique called DSMC is applied to the simulation of the flow feature and evaluation of the main effective term on the performance of the micro gas actuator. The primary objective of this research is to find a scientific overview of both two- and three-dimensional models with experimental results. Meanwhile, effective parameters are recognized to evaluate the main important mechanism for the performance of this micro actuator.

2. Numerical approach

2.1. Governing equations and solver

Molecular method of the kinetic gas theory is known as a consistent and vigorous technique for simulating the

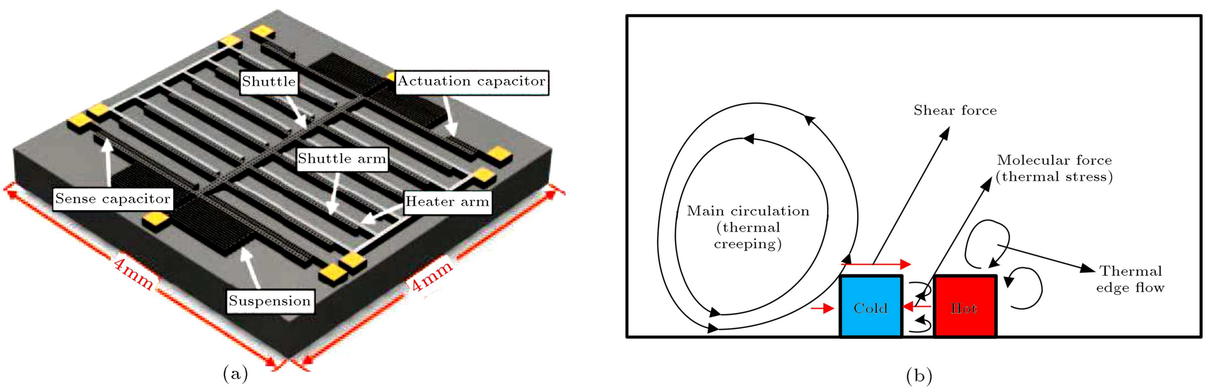

Figure 1. (a) Microscale In-plane Knudsen Radiometric Actuator (MIKRA) device [23] and (b) schematic of flow inside the Micro-Electro-Mechanical System (MEMS) actuator.

model. In this study, the Boltzmann equation was chosen as the governing equation. Several techniques are available for solving the Boltzmann equation. Among various approaches, the DSMC method of Bird [54] is reliable and robust in low-pressure conditions and is a vigorous technique for the molecular system. In the present work, open-source *dsmcfoam* code of the OpenFOAM was applied to take advantage of a skillful employment of difficult models [55]. A number of previous researchers have applied the computational approach to simulating engineering problems [56–62].

2.2. Numerical procedure

In order to model collision in the present study, the Variable Hard Sphere (VHS) collision model was used. Hence, collision pairs were selected according to the no time counter scheme, wherein the run time corresponded to the number of simulated particles [17].

In the proposed model, the size of the gap is the specific characteristic length (L) of the model and it is about 20 M. This study considered $2.48 \times 10^{+5}$ as the total number of simulated particles. According to the molecular characteristics, the time step was calculated and 1×10^{-8} (s) was chosen for our simulations. In this research, cell size, number of particles in each cell, umber of time steps, number of samples, and number of grids were 4 μm, 20, $3 \times 10^{+6}$, and 9910, respectively.

2.3. Geometry and boundary condition

Due to physic of the problem, adopting a two-dimensional approach to simulating the current problem is a reasonable assumption. Figure 2(a) illustrates the chosen domain along with the generated grid. As shown in the figure, the two-dimensional model is just a section of the three-dimensional real model.

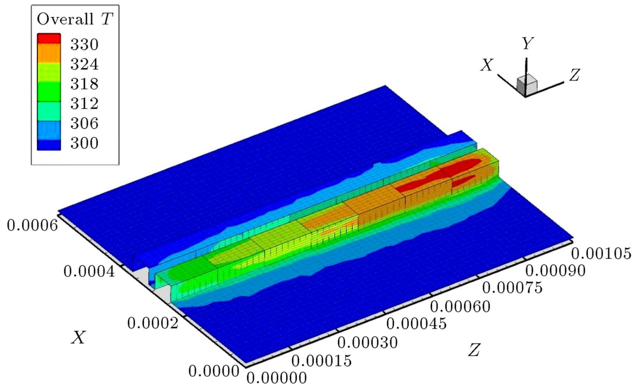

Figure 3. Linear temperature profile of the hot arm in the 3D model.

As shown in Figure 2(a), the full border of the domain is the supposed wall with a fixed temperature. In our work, the performance of this micro gas sensor was examined in a wide pressure range of 62 Pascals to 1500 Pascals, corresponding to Knudsen numbers of 4.64 to 0.19, respectively. Obtained results were also validated with experimental data [23]. In order to apply the real temperature condition of experimental tests to the proposed model, a linear temperature profile was added to the three-dimensional model. Figure 3 clearly illustrates the temperature distribution inside the main 3D model.

3. Results and discussion

3.1. Validation

In order to recognize and evaluate the obtained results, exerting a net force on the cold and hot arms in case of two temperature profiles was investigated using the 3D model. In the main experimental examination [23],

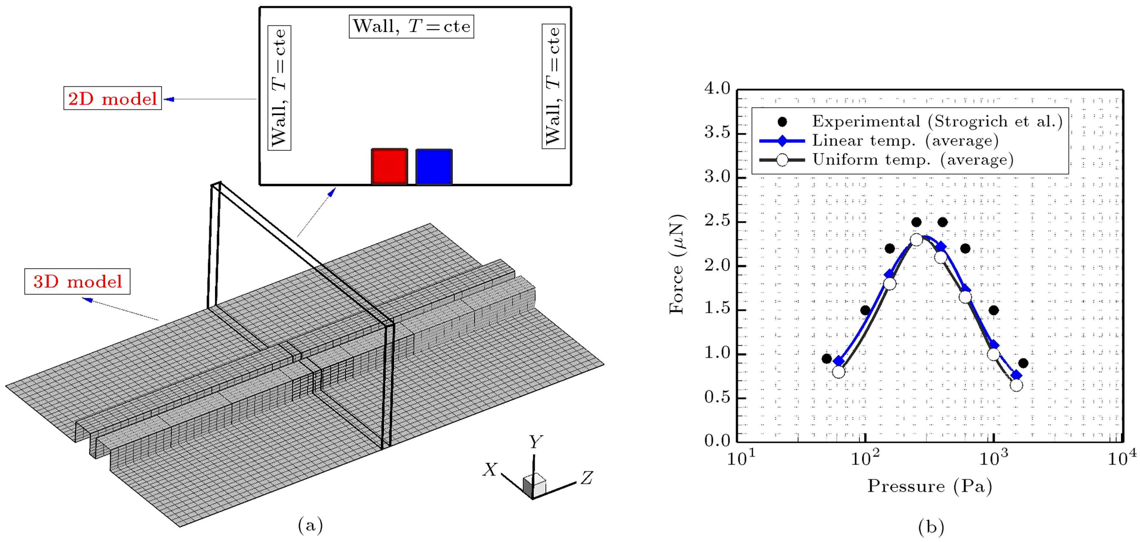

Figure 2. (a) The boundary condition and grid of the present model and (b) comparison of the obtained results (dsmcfoam) and experimental and numerical findings of Strongrich et al. [23] for N_2.

the temperature of the hot arm varied significantly and the maximum and minimum temperatures of the hot arm were presented. In this study, the linear profiles of uniform and average temperatures were applied to the hot arm. Figure 3 illustrates the temperature distribution on the hot and cold arms upon applying a linear temperature profile to the hot arm.

Figure 2(b) shows the comparative results of our 3D simulation and those of experimental examinations for nitrogen gas. The comparison clearly shows that both models present reasonable results with good agreement with experimental data.

In order to evaluate the effect of different collision models, results of Knudsen force applied to the cold arm with VHS were compared with those of soft-sphere and Sutherland potentials, as shown in Table 1. According to the obtained results, the maximum deviation of these models with VHS was less than 6%. Indeed, the model of hard sphere collisions is subject to some deviations when the temperature gradient is high in the proposed model. Since the temperature gradient of the proposed model is limited and less than 50 degrees, the scheme of hard sphere collisions achieved reliable results.

3.2. Flow pattern inside the micro actuator

Since the main particle interactions in our model occur in-plane, the in-plane two-dimensional approach can clearly show the major flow properties inside this micro actuator. Figure 4 shows the flow patterns and temperature distribution of different pressure levels. In these models, the average temperature was applied to the hot arm and thus, temperature varied at different pressures.

In the first overview, the main modification to these models was temperature distribution and it considerably influenced the flow pattern. The circulation of flow on the top of the cold arm significantly shrank as the pressure of the domain increased. Meanwhile, the temperature gradient remained quite limited in the vicinity of the arms. This induces numerous small circulations in the area of the top of hot arms. Indeed, the non-homogeneity of the particles constrains the molecular transmission in the domain. Previously, scholars have introduced the phenomenon of thermal transpiration, which is the main driving mechanism for production of force on Knudsen pumps [56–57]. Computational approaches are widely used in scientific researches [58–75].

Table 1. Knudsen force on the cold arm in different collision models.

Pressure (Pa)	VHS	Soft-sphere	Sutherland
62	0.927	0.882 (+3 %)	0.927(–2 %)
155	1.785	1.632(+5 %)	1.785(–4 %)
387	2.332	2.079(+6 %)	2.332(–5.5 %)
966	1.632	1.552(+2 %)	1.632(–3 %)

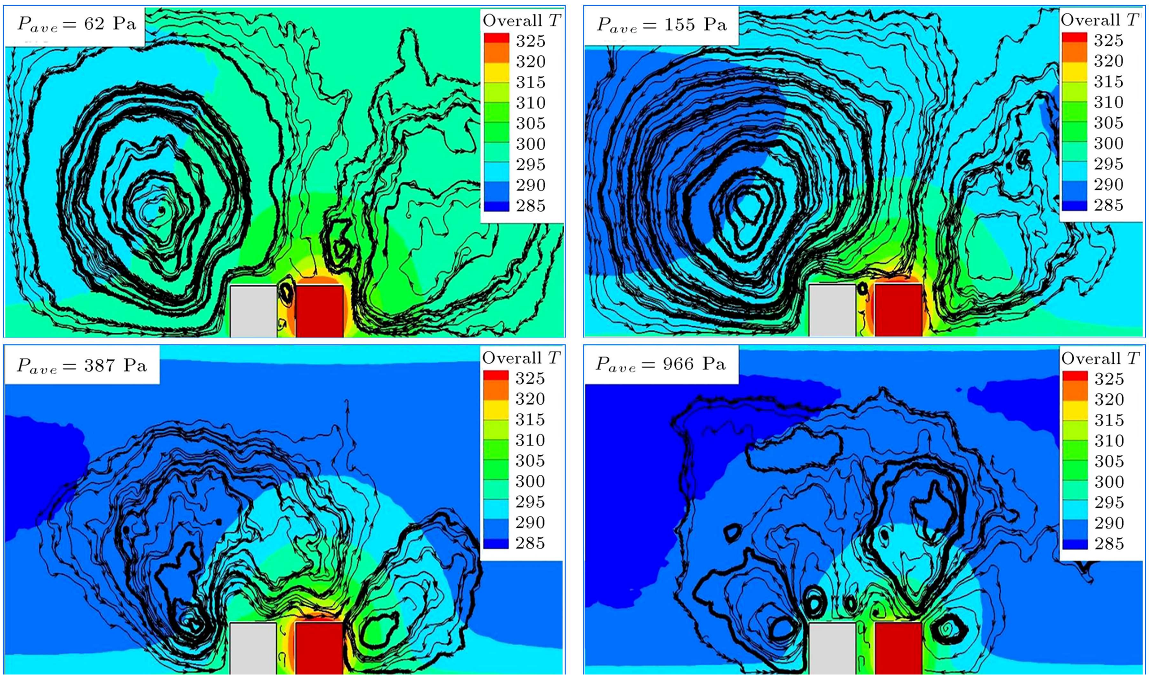

Figure 4. Comparison of the flow feature and temperature distribution in the 2D model.

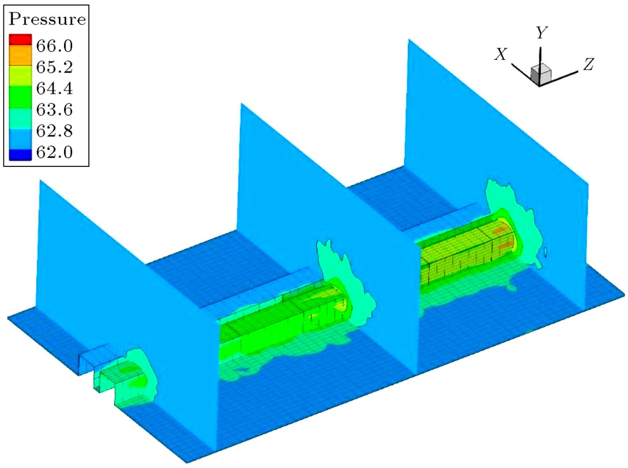

Figure 5. Pressure distribution along the 3D model at $P = 62$ Pa.

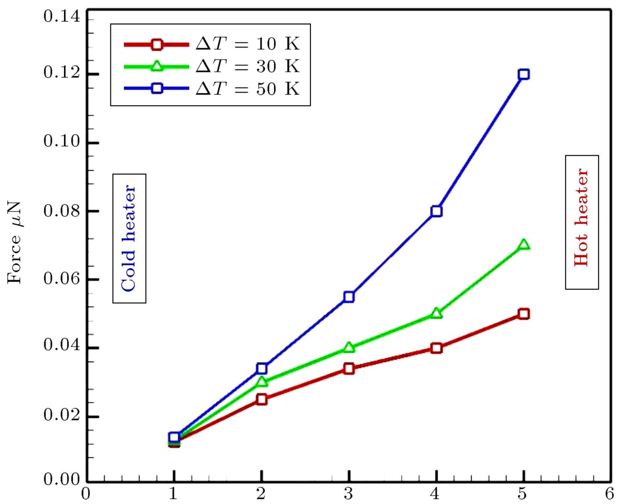

Figure 6. Comparison of the average temperature difference on the Knudsen force along the depth of the cold arm.

Figure 5 depicts the pressure distribution in three cross-sections of the three-dimensional model for domain pressure of 62 Pa. In the three-dimensional model, the pressure gradient clearly varies as the temperature of the hot arm changes.

3.3. Effect of hot arm temperature

Figure 6 illustrates the effect of the fixed temperature gradient on the Knudsen force in a three-dimensional model at a pressure of 387 Pa. According to the figure, the rise of the average temperature of the hot arm significantly increases the Knudsen force in the vicinity of the hot heater. In fact, the major effect of the temperature can be seen in the region where the temperature of the hot and cold sides is considerably different.

Figure 7 shows the pressure and temperature gradient in our domain at $P = 387$ Pa for various sections of the three-dimensional model.

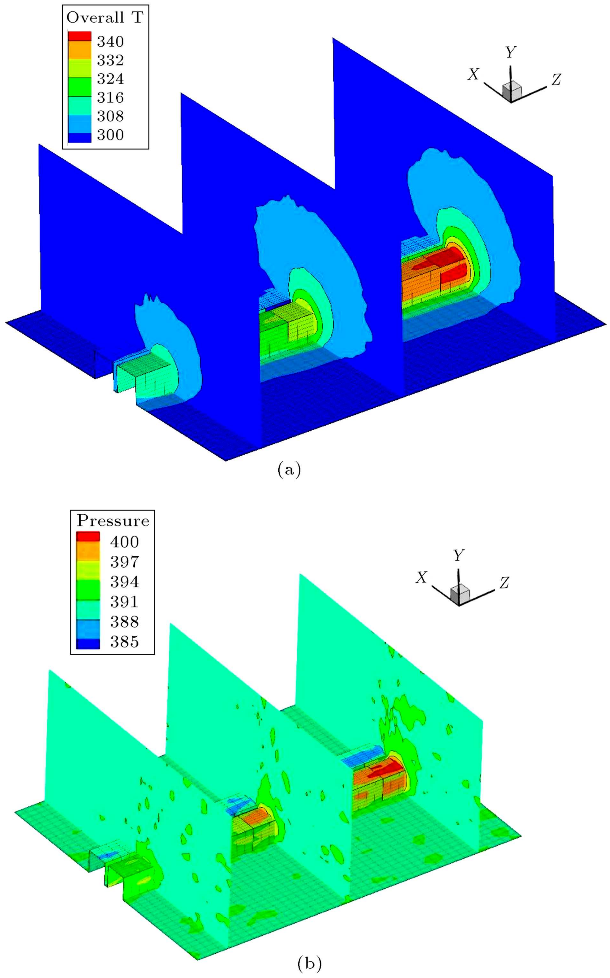

Figure 7. Comparison of (a) Temperature and (b) pressure along the depth of the arm at $P = 387$ Pa.

4. Conclusions

In this study, comprehensive three-dimensional simulations were carried out to investigate the performance of the micro actuator of Microscale In-plane Knudsen Radiometric Actuator (MIKRA) in various conditions. To this end, Direct Simulation Monte Carlo (DSMC) approach was applied to simulating the rarefied gas within this micro sensor. This paper studied the effect of significant parameters such as temperature difference, gap size, length and depth of arm, and operating pressure on the main mechanism of the Knudsen force production inside the rarefied gas. Our findings clearly demonstrated that the effect of gap size and length of arm was greater than other parameters when the temperature difference of hot and cold arm was high.

Acknowledgments

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Biographies

Huawei Wu has been a Professor of Hubei University of Arts and Science in Xiangyang, China since 2015. He is also the Head of Hubei Key Laboratory of Power System Design and Test for Electrical Vehicle. His research interests are engineering, mathematics, physics and astronomy, energy, computer science, and materials science. He works on different projects in Hubei Innovation Project of Mechatronics and Automobiles.

Rasoul Moradi is an Assistant Professor of Chemical Engineering at Khazar University, Baku, Azerbaijan. He has completed his PhD degree in Chemical Engineering-Nanotechnology at Tehran University, Iran. His researches center around the questions about the application of nanomaterials in performance materials. His research group is focused on the synthesis of highly aligned nanofibers and magnetic nanofluids employed in various cases such as piezoelectric devices, polymeric membranes, smart and responsive materials, sensors, and actuators.

Mostafa Barzegar Gerdroodbary received his BSc degree of Mechanical Engineering in Thermal and Fluid from Mazandaran University in 2007. He received his MSc degree in Aerospace Engineering from Iran University of Science & Technology, Tehran-Iran in 2009. He received his PhD degree from Babol Noshirvani University of Technology, Tehran-Iran in 2019. He is now a lecturer at Babol Noshirvani University of Technology.

Mohamadmahdi Shahbazi received his BSc degree of Electrical Engineering in Electronics from Sharif University of Technology, Tehran-Iran in 2006. He received his MSc degree in Electrical Engineering from Isfahan University of Technology, Isfahan-Iran in 2009. He received his PhD degree from Tarbiat Modares University, Tehran-Iran in 2017. Since 2017, he has been with the Faculty of Engineering, Bu-Ali Sina University, Hamedan, Iran as an Assistant Professor.