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DSMC Simulation of Thermal Transpiration and Accommodation Pumps

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Abstract

The Direct Simulation Monte Carlo (DSMC) technique is employed to evaluate several configurations of thermal transpiration and accommodation pumps. There is renewed interest in these rarefied flow pumping concepts for Micro-Electro-Mechanical Systems (MEMS) due to advances in micro-fabrication. The simulation results are compared with existing data to understand gas-surface interaction uncertainties in the experiments. Parametric studies are performed to determine the effects of Knudsen number and surface temperature and roughness on the maximum pump pressure ratio.

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1 Introduction

The concept of pumping rarefied gases by employing dissimilar surface characteristics is not new. A pump is typically defined as a machine in which energy is added to the fluid to increase the pressure, i.e., there is a driving force to "push" the fluid. The strategy of high Knudsen number (Kn > 1) pumps is to maximize the forward flux of molecules and minimize the backward flux. Since gas-surface interactions dominate in rarefied flows, the surface characteristics define these fluxes. This fact can be strategically used to direct the flow with the proper selection and configuration of the surfaces. The surface characteristics can be dissimilar in temperature or roughness or both. Thermal transpiration pumps are driven by differences in surface temperature; accommodation pumps are driven by the difference in molecular reflection from specular versus diffuse surfaces. These two concepts require suitably arranged geometries and can be combined to

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achieve the maximum possible pressure ratio which indicates pumping capability. Thermal transpiration and accommodation pumps offer the advantages of no moving parts and reliability.

Simulation of these pumping concepts enables us to understand existing data in the literature and to perform parametric design studies for various applications. Although several pump configurations have been tested in the literature, minimal analyses have been performed to understand the operation of these pumps or to optimize their design. Some parameters such as surface roughness are difficult to reproduce experimentally but are well-defined and repeatable computationally. Also, there is renewed interest in thermal transpiration and accommodation pumps for rarefied flows due to advances in micro-fabrication. Traditionally, rarefied flow implied low pressures, i.e., for high Knudsen number, the mean free path was large. Now, a large Knudsen number can be obtained with micron-sized characteristic lengths enabling micro applications as well as macro. Thermal transpiration pumps have been considered for use in fusion reactor fuel cycles, space power, boundary layer control, and Micro-Electro-Mechanical Systems (MEMS). Sandia National Laboratories is currently developing a microscale chemistry laboratory to detect and identify chemical agents. While the gas chromatography column in the system is micron-sized, the pump is on the order of centimeters as there is no commercially available micropump. Further insight into gas-surface interactions which define pump performance is needed to develop these concepts for fabrication.

The Direct Simulation Monte Carlo[1] (DSMC) technique will be used to understand existing data and to perform parametric design studies. Due to the comparable size of the characteristic length and the mean free path of the gas, flow through micropumps can range from rarefied to transitional. Thus, the DSMC technique is an appropriate simulation tool for micropumps as it is accurate for both the rarefied and continuum flow regimes. Our DSMC code[2] can run on parallel computer systems which enables conceptual design simulations to be run in a timely fashion. Several configurations of thermal transpiration and accommodation pumps in the literature will be evaluated. DSMC results will be compared with the data and used to determine the effect of surface roughness and temperature, geometry, and Knudsen number on the pumping effect. In all cases, a closed system will be simulated to compute the maximum attainable pressure ratio for the given conditions.

2 Thermal Transpiration Pumps

Over thirty years ago, Edmonds and Hobson[3] investigated the deviation between pressure ratios determined experimentally and by kinetic theory for thermal transpiration. From kinetic theory, $P_1/P_2=a\ (T_1/T_2)^{1/2}$ where P and T are the pressures and temperatures in reservoirs *1* and *2* (as shown in Figure 1), $T_2 > T_1$, and a=1. Based on their data, Edmonds and Hobson postulated that "a hot molecule entering a cold tube has a greater probability of penetration than a cold molecule entering a hot tube." This was the first of their observations on surface roughness effects on thermal transpiration and their later work suggests that a=1 for diffuse surfaces and a=1.1 to 1.3 for more specular surfaces. Many researchers have since sought to obtain analytical and empirical descriptions of thermal transpiration. Others[4] have compared data to these models with disagreement attributed to different material dependent gas-surface interactions than those used to develop the correlations. For general analyses, a more fundamental description is required. The DSMC technique is suited for this purpose and has been proposed by others to simulate thermal transpiration. Sone et. al.[5] employed the DSMC technique to "clarify the cascade mechanism (of Knudsen)"; Vargo and Muntz[6] recognized the need for DSMC simulation for determining the optimum Knudsen number for operating their compressor cascade.

We have employed the DSMC technique to evaluate the two thermal transpiration pump configurations, Figures 1a and 1b, for the conditions shown in Table 1. Configuration T1 was based on the experiments of Edmonds and Hobson[3] using liquid nitrogen for the cold reservoir, 77.4 K, and room temperature, 295 K, for the hot reservoir. The tube is 2.1 mm in diameter and 40 mm long with helium in the closed system. The DSMC predictions of pressure ratio are shown in Table 1. Kinetic theory predicts a pressure ratio of 1.95. The DSMC results compare well with the data[3] and capture the proper trend with decreasing Knudsen number. Convergence of the DSMC solutions, as indicated by small velocities in the tube, were difficult to obtain for the r-z configurations due to the large variance in cell weights. A different cell weighting strategy or reservoir definition improved convergence. Similar to configuration T1 is the T2 micro-configuration shown in Figure 1b. This system includes two reservoirs of air with a temperature difference of 30 K connected by a 0.1μm wide, 1 μm long channel. The DSMC predicted pressure ratios of 1.04 and 1.03 compare well with the kinetic theory of 1.05 and indicate the pumping effect at this lower temperature difference.

3 Accommodation Pumps

Based on Hobson's observations of the effect of surface roughness on thermal transpiration, he proposed an accommodation pump[7]. Configuration A1 in Figure 1c is Hobson's single-stage accommodation pump which capitalizes on the differences between the diffuse and specular reflections on rough and smooth surfaces, respectively. This configuration was evaluated for the two Knudsen numbers in Table 1. Hobson showed that the pressure ratio between the two end chambers at the same temperature should be a in the previous equation, where the pressure on the diffuse end is higher. DSMC predicted a pressure ratio of 1.14 which is in the a-range of 1.1 to 1.3 observed by Hobson. This is the highest pressure ratio of all the accommodation pump configurations in Table 1.

Based on the same gas-surface interaction physics, Tracy[8] proposed the configurations shown in Figures 1d and 1e which employ heated "active" surfaces to direct molecular scattering. Tracy obtained limited data in a chamber filled with helium at 0.1 mTorr with an active surface of carbonized nickel at 873 K. All other chamber surfaces were 303 K. Flow was directed from the 5 mm wide flat strip active surface through a 5 mm wide, 2 mm high aperture 3 mm below the active surface. For this configuration, Tracy measured a pressure ratio of 1.06 between the bottom and top chambers. The ratio of the DSMC computed number densities, which is equivalent to pressure ratio for constant temperature, is about 1.03. Note that while Tracy used an upper chamber of 22 liters, the simulated volume is 55 times less and thus, the hot director plate influences the average temperature whereas it did not in the experimental setup; that is why we examine number densities rather than pressures. Tracy showed that the pressure ratio increases with increasing surface temperature of the director plate which represents an increased degree of surface specularity. The simulations assumed that the active surface was 100% specular with all other surfaces 100% diffuse and thermally accommodating. For a 100% specular director plate, the surface temperature only affects the energy of the molecules striking the top of the director which is assumed diffuse. No pumping effect was observed by Tracy or computed for a heated, diffuse active surface and no pumping effect was computed for a non-heated, specular surface. Thus, the DSMC simulations indicate that the active surface must be both heated and specular to some degree in order to obtain a pumping effect.

The active surfaces were so difficult to reproduce experimentally, that it was difficult to assess the benefit of different geometrical configurations. Improved performance was measured for the cylindrical director configuration (A3). Results of the DSMC simulations in Table 1 confirm that improved performance is indeed due to the cylindrical versus flat strip director given the same conditions. However, the computed pressure ratio for the cylindrical director is much less than the data perhaps due to the small simulation domain or the director position or incomplete gas-surface interaction models or other uncertainties. Improved gas-surface interaction models could be developed such as the energy dependent surface reflection model postulated by Hobson. Tracy obtained even higher pressure ratios on a multi-stage device.

Hemmerich[9] also applied Hobson's accommodation pump concept using suitably arranged inert hot-rough and cold-smooth surfaces such that molecules are preferably transported in one direction. He proposed individual heat sources and heat sinks, differing from Hobson's common source and sink, as shown in the "maze" configuration A4 in Figure 1f. The "active surfaces" are 900 K, diffuse with the remaining surfaces at 300 K and either 70% or fully specular. The pressure at the right end of the maze is greater than the left end by a factor of 1.01 to 1.03. The surface temperature has a greater effect on the pressure ratio than the surface specularity, i.e., with fully specular "other" surfaces, the pressure ratio is 1.01 and with 70% specular, the pressure ratio is 1.03 with hot spots near the active surfaces as shown by the temperature contours in Figure 1f. The DSMC simulations are necessary for this complex geometry and allow quick evaluation of the surface characteristics on pumping capability.

4 Conclusions

The DSMC technique has been successfully used to simulate rarefied to transitional flows in several thermal transpiration and accommodation pump configurations. Computed pressure ratios compared well with data and/or kinetic theory and gave further insight into the data, e.g., Tracy's accommodation pump with a cylindrical director performs better than with a flat strip director. Parametric studies were performed to evaluate the effects of geometry, surface reflection, surface temperature, and Knudsen number. For almost all configurations, the pressure ratio decreased as the flow became more transitional. The choice of a design configuration depends on fabrication capability, surface material availability, and heating technique. The DSMC code could then be used for final design decisions such as type of gas, specific dimensions, and operating conditions. All of the configurations evaluated herein were single-stage concepts. The DSMC tool is required for more complex geometries, such as the accommodation pumps proposed by Tracy[8] and Hemmerich[9], and for multiple stages and three-dimensional geometries.

5 References

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Table 1: Summary of Simulations

Config.*	D, m	n, #/m^3	Kn	T_{surf}, K	Surf. Refl.	P_2/P_1 DSMC	P_2/P_1 Data
T1	2.1e-3	1.69e20	11	Fig1a	Diff	1.85	1.90
		1.85e21	1.1		Diff	1.65	1.72
		1.85e21	1.1		0.5	1.40	
		2.91e22	0.07		Diff	1.09	1.17
T2	0.1e-6	2.38e23	67	Fig1b	Diff	1.04	1.05
		2.38e25	0.67		Diff	1.03	1.05
A1	2.1e-3	6.55e16	35e3	Fig1c	Diff/ Spec	1.14	1.1 - 1.3
		6.55e19	35			1.13	
A2	5e-3	3.03e18	320	873	Diff	1.00	1.0
		3.03e18	320	303	Spec	1.00	--
		3.03e18	320	573	Spec	1.03	--
		3.03e18	320	873	Spec	1.03	1.06
		3.03e18	320	1173	Spec	1.03	--
		3.03e20	3.2	873	Spec	1.01	--
		3.03e21	0.32	873	Spec	0.97	--
A3	5e-3	3.03e18	320	873	Spec	1.07	1.32
		3.03e20	3.2	873	Spec	1.06	--
		3.03e20	3.2	873	0.5	1.07	--
A4	50e-6	3.03e18	32e3	900/ 300	Diff/ 0.7	1.02	--
		3.03e20	320	900/ 300	Diff/ 0.7	1.03	--
		3.03e20	320	900	Diff/ Spec	1.01	--

* See Figure 1

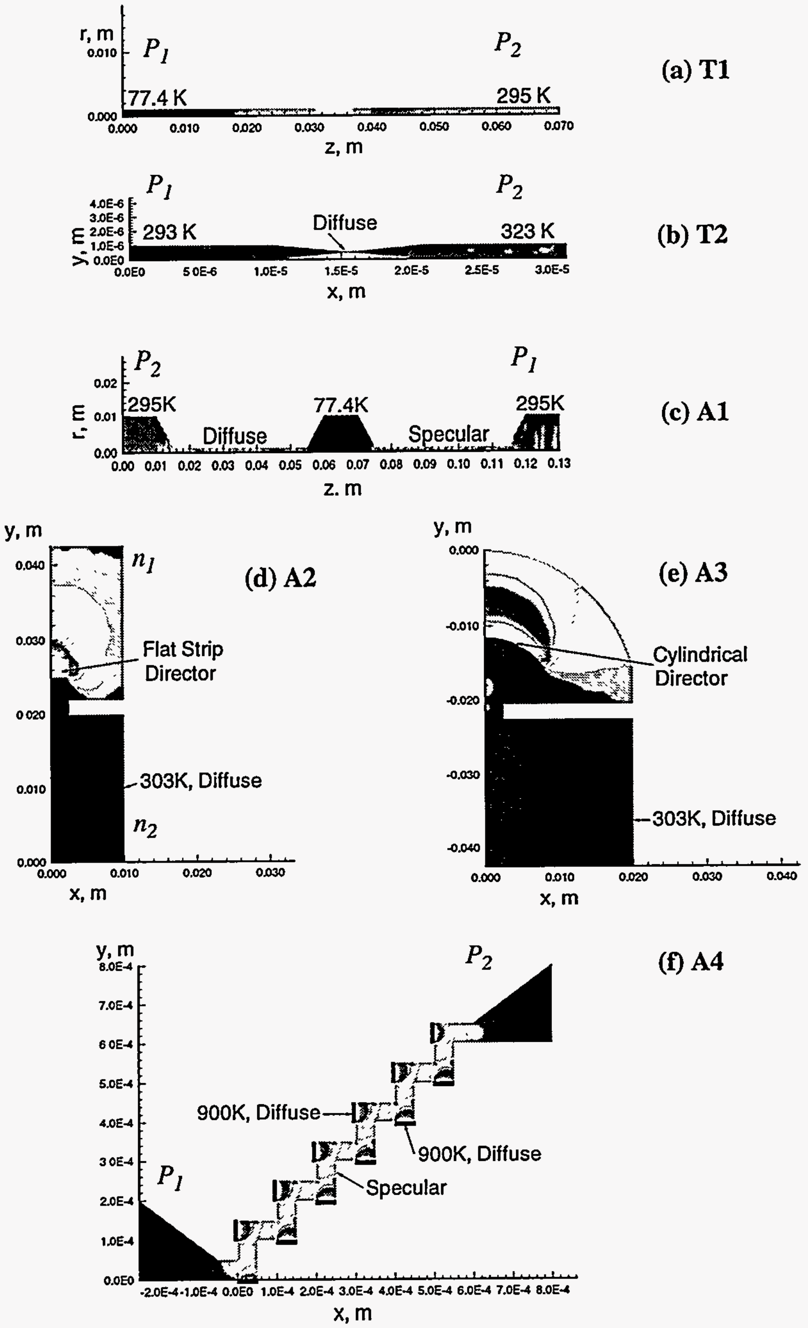

FIGURE 1. Configurations of Thermal Transpiration and Accommodation Pumps