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DESIGN AND MODELLING OF KNUDSEN MICROPUMPS FABRICATED VIA ADVANCED LASER MANUFACTURING

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ABSTRACT

Knudsen pumps are promising candidates for gas pumping in a variety of scientific and industrial applications involving MEMS devices for hydrogen transfer, gas chromatography, aerosol sampling, heat pumps, biomedical systems and sensors etc. These pumps exploit the phenomenon of thermal transpiration, where gas under rarefied conditions flows along a channel due to temperature gradient. This enables gas transport without moving parts, resulting in vibration-free operation, an important feature for miniaturized applications [1].

For applications operating at atmospheric pressure, creating optimal rarefied conditions requires submicron-diameter channels, which is technically challenging. Only a few Knudsen pump prototypes have been reported in the literature, most of which are fabricated using Deep Reactive Ion Etching (DRIE) [2], wet etching [3], or porous materials [4]. DRIE enables the fabrication of channels with dimensions down to 1 μm , but with low aspect ratios (length/diameter ≈ 20) which impose constraints on thermal management. Porous materials contain natural defects that can restrict gas flow and reduce efficiency.

In this work, two Knudsen pumps for over- and sub-atmospheric applications were modeled and designed, taking into consideration the manufacturing capabilities of advanced laser fabrication techniques based on Bessel beams [5] and Selective Laser-Induced Etching (SLE) [6]. Bessel beams enables fabrication of high length-to-radius ratio (>100) nanochannels with diameters down to few nanometers and high writing speeds up to 1000 channels per second. SLE enables the fabrication of precise 3D structures and channels with length-to-radius ratios greater than 50 and diameters down to 3 μm .

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Design

The proposed Knudsen pumps were designed within a 2×2 cm² footprint, ensuring effective thermal management and structural stability. Figure 1 shows a 3D CAD model of the Knudsen pump, illustrating the glass plate (500 μm thick for Bessel beam fabrication and 100 μm thick for SLE fabrication) with through-wafer micro- or nano-channels and integrated heaters on top, as well as the 500 μm thick silicon-based heat sink with micro-pillars on top and 80 μm diameter through-wafer openings. The 1×1 cm² central region is covered by channels, while the surrounding area is reserved for heater and heat sink connections. In the active 1 × 1 cm² region, 600 nm diameter nanochannels (for Bessel beam fabrication) and 3 μm diameter microchannels (for SLE fabrication), etched through the glass thickness, are arranged in a hexagonal pattern with a 20 μm spacing. This configuration results in approximately 300,000 channels.

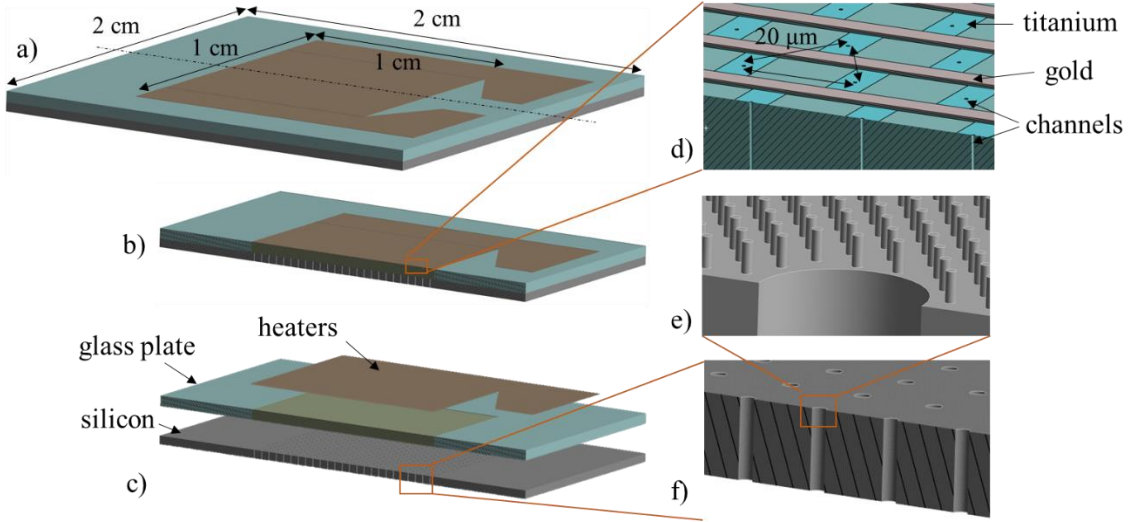


Figure 1: Knudsen pump design: a) complete design, b) half-section view, c) heaters, glass plate and silicon heat sink layers, d) magnified view of the heaters and channels, e) magnified view of the silicon pillars and f) magnified view of the silicon wafer with 80 μm diameter openings.

Gas flow modelling

To optimize the Knudsen pump architecture in terms of channel dimensions and operating pressures, the thermal transpiration flow through a single circular channel was modeled using kinetic theory. Assuming a large length-to-radius ratio (>50), the mass flow rate \dot{m} and pressure distribution $P(z)$ along the channel $z \in [0, L]$ were computed based on the infinite capillary theory. The governing eq. (1)

$$\frac{dP(z)}{dz} = -\frac{v_0(z)}{\pi R^3 G_P(\delta)} \dot{m} + \frac{P(z) G_T(\delta)}{T(z) G_P(\delta)} \frac{dT(z)}{dz}, \quad (1)$$

where $v_0(z)$, R and $T(z)$ are the most probable speed, radius and temperature distribution, respectively, incorporates the Poiseuille G_P and thermal creep G_T flow coefficients, obtained from the linearized Shakhov kinetic model under diffuse boundary conditions [7]. The gas rarefaction parameter, defined as

$$\delta(z) = \frac{P(z)R}{\mu(z)v_0(z)} \quad (2)$$

characterizes the flow regime, where the dynamic viscosity $\mu(z)$ depends on temperature. Numerical solutions of eq. (1) allow computation of either mass flow or outlet pressure for given inlet conditions and temperature gradients. Parametric studies with nitrogen gas identified $R = 0.3 \mu\text{m}$ as the optimal channel radius at atmospheric pressure, and 21 kPa as the optimal operating pressure for $R = 0.15 \mu\text{m}$, to get the maximum pressure difference. For practical applications, the flow characteristics of a single channel are often insufficient. Therefore, pump designs incorporate multiple parallel channels and stages to increase the total mass flow rate and pressure difference, respectively.

Heat transfer modelling

To optimize the temperature gradient across the glass thickness, corresponding to the channel length, heat transfer simulations were performed in ANSYS Mechanical, considering the placement, dimensions, and materials of heaters and heat sinks. Larger temperature differences enhance mass flow rate and pressure difference in thermal transpiration. Materials with lower thermal conductivity produce larger temperature gradients, supporting the choice of glass for channel fabrication. Heaters are applied to one side of the glass, while heat sinks efficiently dissipate heat from the opposite side. Thin gold-titanium layers enable Joule heating, and silicon heat sinks provide high thermal conductivity, mechanical stability, and compatibility with glass for bonding. Silicon pillars around each channel maximize temperature gradients while allowing gas flow, refining the thermal design of the pump.

Fig. 2 shows the results of heat transfer simulations of the designs presented in Fig. 1. They demonstrate that integrating heaters and heat sinks around each of the 300,000 channels produces: a) an average ΔT close to 47 °C for the Bessel beam design when 10 W of heating power is applied, and b) an average ΔT of about 20 °C for the SLE design when 20 W of heating power is applied, while maintaining a maximum temperature on the top side of the glass below 110 °C. The smaller ΔT in the case of SLE is due to the significantly thinner glass compared to the case of Bessel beams. However, the simulations indicate that increasing the channel density, i.e., packing the channels closer together, can enhance ΔT . These results confirm the effectiveness of the proposed thermal management strategy, enabling high-performance and compact Knudsen pump operation.

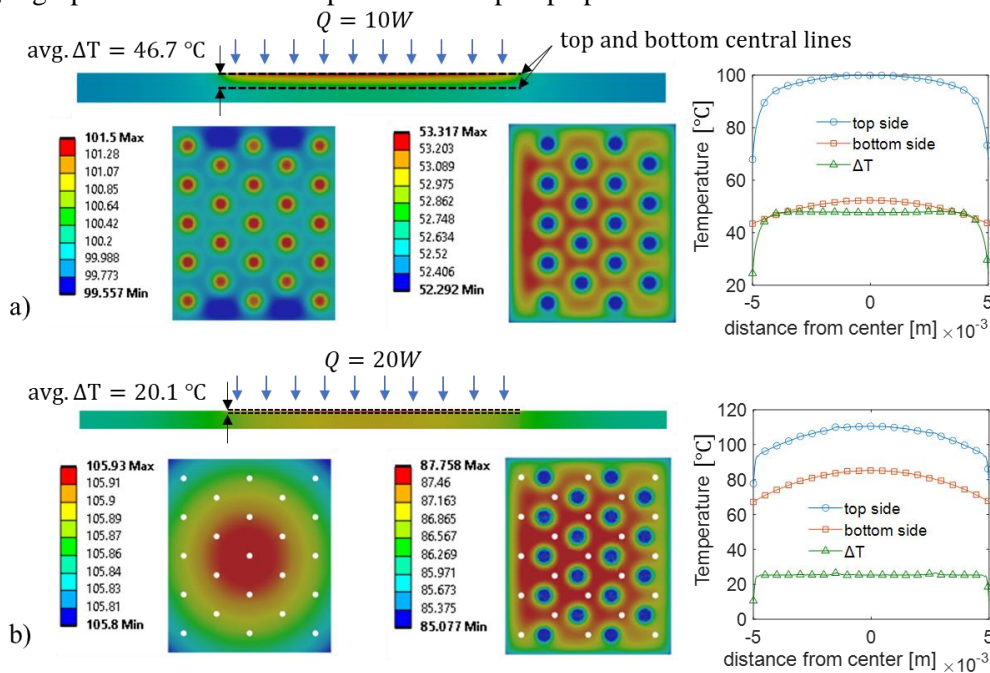


Figure 2: Thermal simulations results of the a) Bessel beams pump and b) SLE pump, showing the cross-sectional view, detailed views of the glass top beneath the heaters (on the left) and the glass bottom above the pillars (on the right), as well as the temperatures along the central line on the top and bottom glass surfaces and the corresponding ΔT graph on the right).

Performance study

In both Knudsen pump designs, the temperature gradients vary across channel positions, even under uniform heat flux on the top surface. Channels experiencing higher ΔT generate larger mass flow rates and pressure differences, while channels with lower ΔT can induce reverse flow. To model this behavior, an iterative scheme was developed for single-stage pumps, calculating the total mass flow and pressure difference by accounting for the individual temperature differences of each channel. A key finding is that using the average ΔT across all channels provides results in excellent agreement with simulations that apply different ΔT values for each channel. For the Bessel beam design with 300,000 channels, an average ΔT close to 47 °C yields a maximum mass flow of $3.5 \times 10^{-10}\text{ kg/s}$ and a pressure difference

of 1575 Pa. For the SLE design, the average ΔT of about 20 °C produces 2.46×10^{-8} kg/s and 72 Pa. For both pumps, atmospheric conditions were applied as initial conditions. Using upstream and downstream volumes of 86 mL, the maximum ΔP is reached within 3 hours with the Bessel beam pump and within 5 seconds with the SLE pump. The algorithm has also been extended to multi-stage pumps, enabling realistic simulation of gas flow through parallel channels and multiple stages. Fig. 3 presents the characteristic curves of the single-stage pumps for their optimal conditions (100 kPa for Bessel beams and 21 kPa for SLE) and at higher pressures, as well as the results of the multistage configuration of these two pumps at atmospheric inlet conditions. With 150 stages in the Bessel beams pump and 1800 stages in the SLE pump, pressure differences of 2 bar and 1 bar were achieved, respectively. It is observed that the Bessel beams pump can provide much higher pressure differences while the SLE pump much higher mass flows. Therefore, the most suitable pump can be selected based on the intended application.

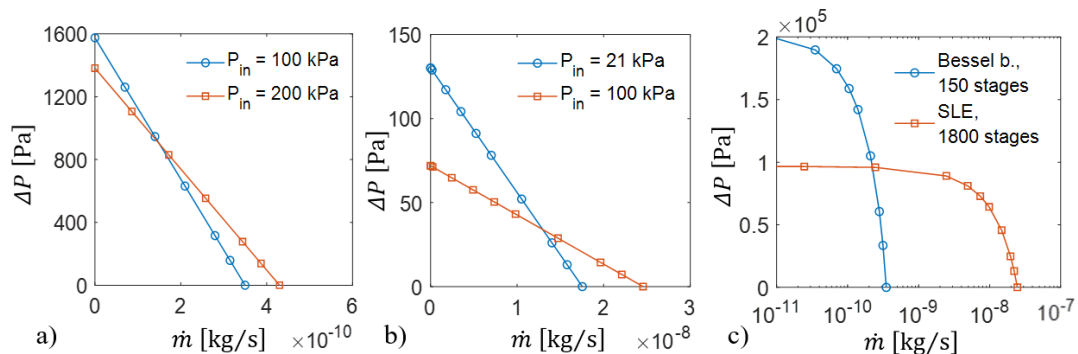


Figure 3: Characteristic curves of the single-stage pumps: a) the Bessel beam case, b) the SLE case, and c) the multistage operation of both pumps.

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