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## Analysis of flow induced by temperature fields in ratchet-like microchannels by Direct Simulation Monte Carlo



Jie Chen<sup>a</sup>, Stefan K. Stefanov<sup>b</sup>, Lucien Baldas<sup>a</sup>, Stéphane Colin<sup>a,\*</sup>

<sup>a</sup> Institut Clément Ader (ICA), Université de Toulouse, CNRS-INSA-ISAE-Mines Albi-UPS, Toulouse, France <sup>b</sup> Institute of Mechanics – BAS, Acad. G. Bontchev St., bl. 4, 1113 Sofia, Bulgaria

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#### ABSTRACT

This paper presents a numerical analysis of a novel configuration of Knudsen pump for rarefied gas flow. The pumping element consists of two facing isothermal ratchet surfaces at different temperatures. The asymmetric saw-tooth-like surfaces in optimal geometric conditions can create temperature inequalities in the near wall region and finally engender a macroscopic flow. The rarefied gas flow is numerically investigated by Direct Simulation Monte Carlo (DSMC) in the slip and transition regimes. A parametric study reveals the effects of several crucial parameters including temperature difference, Knudsen number, accommodation coefficients as well as main geometrical parameters. In particular, the results indicate that the mass flow rate reaches a maximum value for a Knudsen number around 0.1 and becomes negative for a Knudsen number close to unity.

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### 1. Introduction

In rarefied gases, flows can be generated by a tangential temperature gradient applied along a wall without any initial pressure gradient. This well-known phenomenon is the so-called thermal transpiration (or thermal creep) effect. It is the basis of the Knudsen pump operation principle, which allows gas pumping without any moving part when the gas is under rarefied conditions. This kind of pump could provide reliable and precise control of gas microflows for a variety of applications, such as gas-sensing breath analyzers, chemical weapons detectors or micro vacuum generators directly integrated in MEMS. Following the seminal work of Knudsen [1], several different designs of Knudsen pumps have been studied in the past years. The typical Knudsen micropump is based on a cascade system in which a basic unit is composed of a microchannel [2–4] or a microporous medium [5,6] connecting two mini chambers with different temperatures. An alternative configuration has been proposed and numerically studied, consisting of alternately connected curved and straight microchannels [7-9] or curved microchannels with different curvature radii [10]. A thermal edge compressor has been devised and experimentally investigated by Sugimoto [11]. This compressor includes an array of unheated plates made in ceramic that are facing an array of heated plates made of a Nichrome ribbon heater.

two facing isothermal surfaces at different temperatures, one of which at least being unsymmetrically nanostructured, has recently been proposed and studied [12-14]. This so-called "ratchet micropump" is composed of isothermal surfaces at two different temperatures. The major advantage of this type of Knudsen pump is that the temperature gradients within the gas along the walls result from the specific structuration of isothermal walls rather than from a non-uniform temperature distribution along the solid walls. Consequently, the fabrication and temperature control of a ratchet pump are much easier than those of conventional Knudsen pumps, which require a periodic temperature distribution with temperature gradients along the microchannels and opposed temperature gradients in mini chambers. In all cases, heated and cooled zones of very small areas are usually required to achieve the appropriate periodic temperature distribution. The influence of the area of these heated and cooled zones has been numerically investigated for a micropump based on alternately connected curved and straight micro-channels [9] and practical limitations have also been described. Moreover, the control of temperature becomes more complicated when more stages are used to create a more powerful pump. In contrast, the heating/cooling system of a ratchet pump is relatively convenient to design. A multi-stage ratchet pump with increased power could be easily manufactured by simply using surfaces with several ratchet elements, without adding issues linked to temperature control.

A new promising configuration of Knudsen pump consisting of

<sup>\*</sup> Corresponding author. E-mail address: stephane.colin@insa-toulouse.fr (S. Colin).

Symbols c <sub>r</sub> d	relative velocity of colliding molecules	u v Va	velocity in <i>x</i> -direction velocity in <i>y</i> -direction
EN EN	number of real molecules represented by a test	x	Cartesian coordinate (streamwise direction)
- 11	molecule	v	Cartesian coordinate (spanwise direction)
h	distance between the planes of the ratchet tips	5	
$h_0$	smallest distance between two walls in the $y$ -direction	Greek symbols	
Kn	Knudsen number	α	tangential momentum accommodation coefficient
L	characteristic length, ratchet pattern length	β	ratchet angle
$L_m$	misalignment distance between ratchet patterns of	λ	molecular mean free path
	facing walls	$\mu$	dynamic viscosity
Ν	number of test molecules	$\sigma_T$	collision cross section
$N_{C}$	maximum collision number		
n	normal coordinate	Subscript	
Р	pressure	h	hot wall
Т	temperature	С	cold wall
t	time	V	vertical wall
S	tangential coordinate	Ι	inclined wall

In the original ratchet pump configuration, several special surface boundary conditions have been assumed. For example, a structured surface combining diffusive and specular segments was considered by Donkov et al. [12], who analysed a twodimensional prototype channel which is composed of a cold flat wall and a hot ratchet surface (Fig. 1a). The cold flat wall is parallel to the x-direction and has a diffusive surface, whereas the hot ratchet-structured wall exhibits a periodic geometrical pattern divided into three segments: two diffusive boundary segments in the x- and y-directions linked by one tilted specular segment. Donkov et al. demonstrated that: (i) a net flow rate is thermally generated in the *x*-direction when the gas is rarefied; (ii) there is no momentum in the *x*-direction when the entire structured wall has a diffuse surface and the asymmetry of the wall topography is not a sufficient condition to generate a flow along the channel. Würger proposed a ratchet pump design [13] based on the same physical mechanism as mentioned in [12]. It consists of two facing ratchet surfaces with the same topography maintained at a respectivelv hot and cold uniform temperature (Fig. 1b). Würger developed a simplified analytical model assuming a small ratchet depth *d* (i.e. valid for d < h, where *h* is the distance between the two planes of the ratchet tips). It was demonstrated that velocities of several meters per second could be obtained and that the thermally driven flow phenomenon should also be observed for a larger distance between both plates, up to hundred times higher than the mean free path of the molecules. However, the thermal creep along the vertical wall segments was neglected in Würger's model.

Recently, by means of a Computational Fluid Dynamics (CFD) approach, three of the present authors numerically studied the performance of a new type of Knudsen pump with a misalignment of the upper and lower ratchet patterns (Fig. 1c) [14]. Using the Navier-Stokes equations with appropriate velocity slip and temperature jump boundary conditions, it was demonstrated that the pumping effect could be observed in the slip flow regime. Furthermore, the simulations revealed that the pump could operate even if all segments of the ratchet surfaces are diffusive walls. In other words, the finding emphasized the fact that a working device does not necessarily require, as claimed in [12], the presence of some specular segments, which are not practically achievable, as confirmed by most experimental measurements showing that the tangential accommodation coefficients range in practice from 0.85 to unity [15], which corresponds to rather diffusive wall conditions. Additionally, the influence of the geometric parameters and rarefaction was studied in [14]. It was observed that the mass flow rate increases with the Knudsen number in the rarefaction range corresponding to the slip flow regime. For the highest investigated values of the Knudsen number, the mass flow rate becomes less dependent on the Knudsen number, suggesting that a maximum value is expected in the early transition regime, where the Navier-Stokes based approach is not appropriate any longer.



Fig. 1. Three ratchet designs analyzed by (a) Donkov et al. [12], (b) Würger [13] and (c) Chen et al. [14]. In (a), diffusive walls are represented by dashed lines and specular walls by dotted lines.

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