Investigation of Gas Separation Induced by Thermal Loading

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Abstract- **Gas separation using thermal transpiration is proposed and investigated. In thermal transpiration, rarefied gas flow is driven by thermal loading, and the differing molecular weights in a gas mixture leads to differing flows and therefore separation of the mixture. This approach to separation may be especially applicable in micro- and nanosystems, since the requirement for relatively bulky pumps, typically required in conventional membrane filtration or gas chromatography, is eliminated. In this paper, we report our preliminary investigation of the separation effect caused by a thermal gradient in a mixture gas flow. The dependence of separation performance on various parameters, including temperature loading, molecular weight, and channel size, are investigated.**

INTRODUCTION

When a rarefied gas flow is subjected to a thermal gradient, a variety of non-intuitive "cross effects" can occur. For example, at steady state, a pressure gradient can be established as a result of an applied thermal gradient. Such a phenomenon has been recently utilized in developing "Knudsen" pumps for a variety of applications [1,2]. The fact that no moving parts or lubricants are required makes these pumps particularly attractive in miniaturized micro vacuum systems. In this work, we focus our attention on the cross effects occurring in a gas *mixture*. Under the effects of a thermal gradient, a concentration gradient as well as a pressure gradient can be established. This effect can potentially be used as a separation mechanism for gas mixtures; such separation schemes are in demand for 'on-chip' bio/chemical reactor applications. We report our preliminary investigations of gas separation induced by a thermal gradient in the rarefied flow regime.

BACKGROUND THEORY

When device sizes scale down, the mean-free-path of gas molecules becomes comparable to the characteristic length of the device. A molecular approach is often required to model such micro/nano gases. Based on kinetic theory, the state of the gas can be described by the velocity distribution function of each species which obeys the Boltzmann transport equation [3]. In the absence of external forces, this approach yields:

$$\frac{\partial f_\alpha}{\partial t} + v \cdot \frac{\partial f_\alpha}{\partial r} = \sum_\beta Q(f_\alpha, f_\beta) \cdot \qquad (1)$$

where f_α and f_β refer to the distribution functions of species α and β, respectively, t is the time, r is a vector of spatial coordinates, v is the velocity of the particle and Q is the collision integral between species α and β. Once f is found, macroscopic variables can be calculated based on the density function through averaging.

ANALYSIS AND RESULTS

Referring to Fig. 1, two reservoirs held at two different temperatures are connected by a channel whose length (L) is much larger than its width (W) and its height (H) and $H \leq W$. It is assumed that the longitudinal temperature profile is linear and the dimensionless thermal gradient, defined as $\frac{H}{T}\frac{\partial T}{\partial z}$, is very small. We are interested in finding the resultant steady-state concentration ($C = n_\alpha / (n_\alpha + n_\beta)$, n is the number density) profile as well as the pressure profile along the channel. The solution scheme involves three steps. First, the Boltzmann transport equation (BE) is linearized near the local Maxwellian and kinetic coefficients, as functions of concentration, are found by solving the linearized BE with the McCormack collision model [4]. The requirement of zero mass flux and diffusion flux at steady state allows one to find concentration and pressure gradients at each cross section utilizing the kinetic coefficients and Onsager-Casimir reciprocity relations. Finally based on the mass conservation law, concentration and pressure profiles are found by solving two coupled nonlinear integral equations using Newton's scheme together with numerical integration.

Fig. 2 shows the concentration profiles of a He-Xe mixture in a channel under different thermal loadings. An almost 12% separation has been achieved in both reservoirs at a thermal gradient of 0.0007 ($T_A = 773K, T_B = 273K$). In addition to the thermal loading, another important parameter that affects separation is the molecular mass ratio of the mixture. Fig. 3 shows the concentration profiles of two different mixtures (He-Xe and Ne-Ar). As expected, a greater separation is observed in the mixture of He-Xe whose molecular mass ratio, defined as mass of heavy molecule to mass of light molecule, is higher. It is also interesting to examine the influence of channel dimensions, particularly the height, on the separation. These dimensions dictate the degree of rarefaction and thus the gas transport mechanism. Fig. 4 shows concentration profiles of He-Xe mixture in channels with various heights but the same height-width (H/W) ratio. Fig. 5 shows the same profiles in two channels of the same height but with different height-width ratios. Separation improves slightly in the channel with a smaller H/W ratio. We conclude that with a proper design, thermally induced separation could potentially be an efficient approach for micro/nano scale gas separation.

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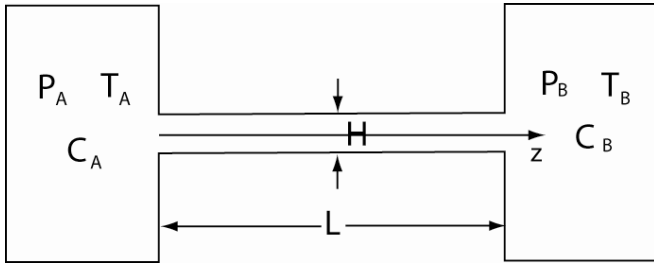
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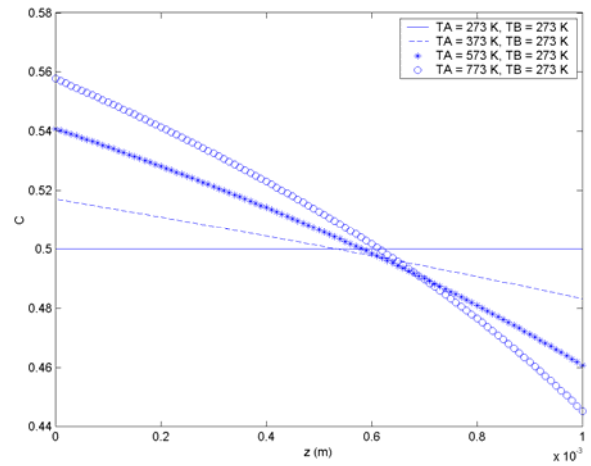Fig. 1. Schematic of two gas reservoirs connected by a channel.

Fig. 2. Concentration profiles of He-Xe mixture along the channel (L = 1 mm, W = 7300 nm, H = 730 nm) at different thermal loadings.
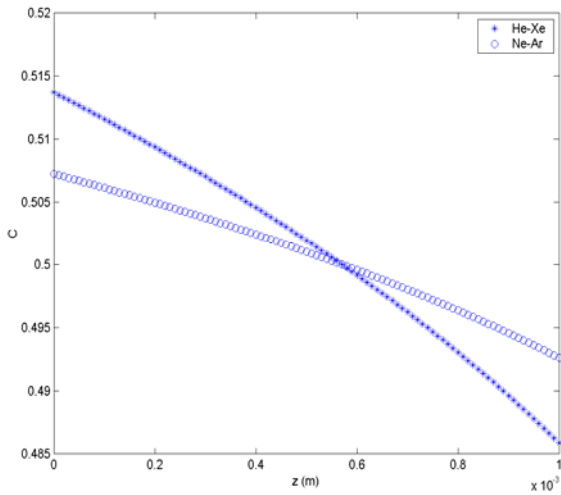

Fig. 3. Concentration profiles of two different mixtures in a channel with L = 1000 mm, W = 730 nm and H = 73 nm. T_A = 573 K and T_B = 273 K.
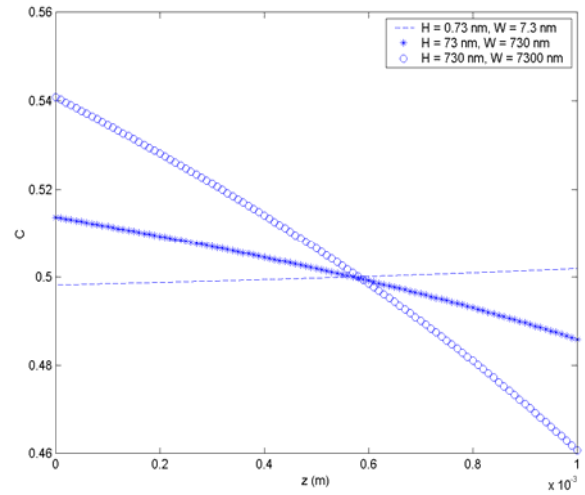

Fig. 4. Concentration profiles of He-Xe mixture in channels with different heights but the same height-width ratio. T_A = 573 K and T_B = 273 K and L = 1 mm.
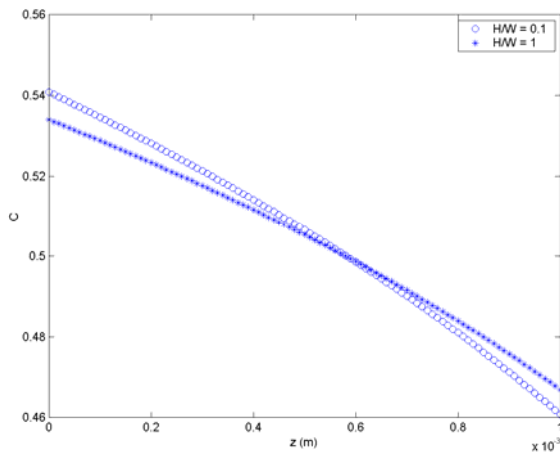

Fig. 5. Concentration profiles of He-Xe mixture in channels with the same height (H = 730 nm) but different height-width ratio. T_A = 573 K and T_B = 273 K and L = 1 mm.