Application of the Gaseous Cross Phenomena to Microfluidics

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ABSTRACT

Since the size of microfluidics is very small the gas flowing through micropumps, microvalves etc. can not be considered as a continuous medium but its rarefaction must be taken into account. The rarefied gas properties are qualitatively different from those of a continuum fluid. The principal different is the existence of the so-called cross phenomena, which can be used to create new types of microfluidics and to optimize the existing ones. For instance, the thermocreep is successfully used in micropumps without moving parts. The light induced drift of gas allows us to move a gas using a laser beam. Many cross phenomena appear in an anisotropic medium such as a polyatomic gas staying in a magnetic field. As a result, the gyrothermal effect arises between two coaxial cylinders confiding a polyatomic gas. The thermal magnetic effect can be also used to pump a polyatomic gas. In the present paper a review of the cross phenomena is given with their numerical estimations when possible.

Keywords: Cross phenomena, Rarefied gas, Microchannels, Micropumps, Microvalves.

1 INTRODUCTION

If we restrict ourselves by the linear region of physical laws all irreversible phenomena can be described in the quite general form

$$J_k = \sum_{n=1}^{N} \Lambda_{kn} X_n , \qquad 1 \le k \le N , \qquad (1)$$

where X_k are thermodynamic forces (e.g. temperature gradient, concentration gradient), and J_k are conjugated thermodynamic fluxes (e.g. heat flux, diffusion flux), and Λ_{kn} are kinetic coefficients. The diagonal coefficients Λ_{kk} describe the direct phenomena. These phenomena are well known, e.g. heat flux caused by a temperature gradient (Fourier's law), diffusion flux caused by a concentration gradient (Fick's law). The non - diagonal coefficients Λ_{kn}, $(k \ne n)$ describe the so-called cross effects, e.g. diffusion flux induced by a temperature gradient, heat flux induced by a concentration gradient.

The above mentioned cross effects exist in continuum regime of flow, i.e. when the Knudsen number Kn=λ/a is very small. Here, λ is the molecular mean free path and a is a characteristic size of the gas flow. However, in rarefied gases, i.e. when the Knudsen number is not small, many new cross phenomena appear, which can be used to create new types of microfluidics or to optimize the existing ones.

A general theory of the cross phenomena in a single rarefied gas is given in the work [1]. Using this theory many specific effects were pointed out in the paper [2]. Then, the theory and its application were generalized for gaseous mixtures [3] and for rotating gaseous systems [4]. The light induced drift of gas [5] is one more cross effect that can be used in microfluidics. This phenomenon allows us to move a gas using a laser beam. Many cross phenomena appear in an anisotropic medium such as a polyatomic gas staying in a magnetic field. As a result the gyrothermal effect [6] arises between two coaxial cylinders confiding a polyatomic gas. This phenomenon can be used to create a new type of micromotor.

The most important property of all cross phenomena is the Onsager - Casimir reciprocity relations [7], [8], which can be formulated as follows: If the set of the thermodynamic fluxes J_n and thermodynamic forces X_n is chosen so as the entropy production in the system is expressed as the sum

$$\sigma = \sum_{n=1}^{N} J_n X_n ,$$

then, the kinetic coefficients satisfy the relations

$$\Lambda_{kn} = \varepsilon_k \varepsilon_n \Lambda_{nk} , \qquad (2)$$

where $\varepsilon_k = \pm 1$ depending whether the corresponding thermodynamic force X_k changes its own sign at the time reversal or it does not. The derivation of the kinetic coefficients Λ_{kn} satisfying the reciprocity relations is not so trivial task as on can think. For some types of the gas flow their expressions are very complicated. But the formalism developed in the papers [1]–[6] allows us to simplify the derivation of the kinetic coefficients.

Why does one need the reciprocity relation? Nowadays, these relations become a very useful tool in engineering. With the help of them one can: (i) predict

new cross phenomena, (ii) reduce numerical efforts in practical calculations, (iii) reduce experimental efforts to measure the kinetic coefficient, (iv) control a numerical accuracy or an experimental error.

Usually the cross phenomena are very small in comparison with the direct ones. But there are many situations when the direct effects vanish and the cross ones dominate.

To calculate the kinetic coefficient Λ_{kn} the Boltzmann equations

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\Gamma}\frac{\partial f}{\partial \Gamma} = Q(ff_*) \qquad (3)$$

must be solved. Here, $f = f(t, \mathbf{r}, \Gamma)$ is the one-particle distribution function, t is the time, $\mathbf{r}$ is the position vector and Γ is the set of variables describing the state of one molecule (velocity, angular moment, quantum state etc.), $Q(ff_*)$ is the collision integral. On the solid surface some boundary conditions are assumed, e.g. the diffuse reflection of the gaseous molecules.

The numerical solution of the Boltzmann equation is very difficult task that is why many model equations are applied in practical calculations. To obtain reliable numerical results the model equation must be thoroughly chosen. The choice depends on the type of gas (monoatomic or polyatomic) and on the thermodynamic forces taken into account. As was shown in the review [9] to calculate the non-isothermal gas flow the so-called S model must be applied instead of the usually used BGK model.

The aim of the present paper is to give a review of the cross phenomena existing in rarefied gases with their numerical estimation when possible.

2 THERMAL CREEP

2.1 Definition

The thermal creep, i.e. the gas flow through a capillary caused by a temperature gradient, is most studied cross phenomenon arising in rarefied gases. An extensive list of the papers on the effect with a critical analysis and recommended data can be found in the review [9]. This phenomenon can be used for micropumps without moving parts. Moreover, the effect allows us to supply microquantities of a gas. Changing the temperature gradient one can control the quantity of the supplied gas. Here, it must be note that the gas flows from the "cool" reservoir staying at the lower temperature to the "hot" one staying at the higher temperature.

The cross phenomenon coupled with the thermal creep by the reciprocity relation (2) is the mechanocaloric effect, i.e. the heat flux caused by a pressure gradient. This effect has not a practical application, but because of its coupling with the thermal creep it is very useful for theoretical analysis, e.g. the data given below were calculated via the mechanocaloric effect.

It should be noted that quantitatively the thermal creep for monoatomic gases differs from that for polyatomic ones. The data presented below were obtained for monoatomic gases, i.e. the set of the variables Γ of the distribution function contains only the molecular velocity. The flow rate for a polyatomic gas must be calculated including the angular moment of molecules into the set Γ.

2.2 Capillary flow

Let us consider a cylindrical capillary connecting two reservoirs, which contain the same gas. A pressure P is maintained in both reservoirs, i.e. there is no pressure drop, but there is a temperature drop on the capillary ends. Let T_0 be the temperature in the left container and T_1 be the temperature in the right one.

The numerical data on this effect, usually, is given in dimensionless form, e.g. the reduced flow rate G_T is presented as a function of the rarefaction parameter $\delta = 2\lambda/(\sqrt{\pi}a)$, where a is the capillary radius. To have an idea on the order of the flow rate, here some dimension data are given for the temperature ratio $T_1/T_0 = 3.8$. This ratio is realized when one reservoir is staying at the room temperature $T_1 = 293$K and the other reservoir is staying at the liquid nitrogen temperature $T_0 = 77.2$K.

Using the data on the coefficient G_T, (Ref.[10], Table V) one can calculate the flow rate M (mole per second) as

$$M = 69.1\frac{a^3(T_1 - T_0)\,P\,G_T}{\ell(T_1 + T_0)^{3/2}m^{1/2}},$$

where ℓ is the capillary length, m is the atomic mass of the gas. In Table 1 the numerical data on the flow rate M for the helium gas is given as function of the capillary radius a and of the gas pressure P. It is assumed $\ell = 10a$.

One can see, with the increasing pressure the value of the flow rate M increases too. But the quantity M reaches its maximum value and then it does not depend on the pressure more. It is explained by the fact that the reduced flow rate G_T is proportional to the Knudsen number in the hydrodynamic regime (Kn $\ll$ 1). But the Knudsen number is inversely proportional to the pressure. Since the quantity M contains the product PG_T, it does not depend on the pressure. Using the asymptotic expression of G_T at Kn $\ll$ 1 one easily obtains the expression of maximum value of the flow rate for any given temperatures T_0 and T_1 and for any monoatomic gas

$$M = \frac{4.7a^2\mu(T_0)(T_1^{3/2} - T_0^{3/2})}{\ell(T_1 + T_0)T_0^{1/2}},$$

where $\mu(T_0)$ is the gas viscosity at the temperature T_0. The independence of the flow rate M on the pressure

Table 1: Mass flow rate M for helium through a capillary vs radius a and pressure P

a [μ]	$M \times 10^9$ [mol/s]		
	P=0.01 [atm]	0.1	1
0.5	0.022	0.15	0.50
1.0	0.081	0.48	1.2
2.5	0.44	1.9	3.2
5.0	1.49	5.0	6.6
10.	4.8	12.	13.
50.	50.	66.	67.

Table 2: Mass flow rate M for helium through a channel vs height a and pressure P

a [μ]	$M \times 10^9$ [mol/s]		
	P=0.01 [atm]	0.1	1
0.5	0.17	0.91	3.0
1.0	0.59	2.8	7.1
2.5	2.9	11.	20.
5.0	9.1	30.	42.
10.	28.	71.	85.
50.	298.	415.	424.

in the hydrodynamic regime can be used for a precise control of the quantity of the supplied gas.

2.3 Channel flow

Let a channel connect two reservoirs having the same pressure P, and the different temperatures T_0 and T_1. Let us denote the channel height as a, its width as b and its length as ℓ. The reduced flow rate G for such type of the flow at T_1/T_0=3.8 given in the work [11] is related to the flow rate (mole per second) as

$$M = 7.78 \frac{a^2 b \, P \, G}{\ell \, (m T_0)^{1/2}}.$$

In Table 2 the quantity M for the helium gas is given as a function of the height a and of the pressure P. It is assumed that a/b=0.05 and $a/\ell = 0.1$. One can see that for the large values of a and P the flow rate M also weakly depends on the pressure. In the hydrodynamic regime (Kn $\ll$ 1) we have the following expression for the flow rate M of any monoatomic gas through a channel with an arbitrary ratio a/b

$$M = \frac{1.47 \, a \, b \, \mu(T_0)(T_1^{3/2} - T_0^{3/2})}{\ell(T_1 + T_0)T_0^{1/2}}.$$

This is the maximum value of the flow rate M at the given temperatures T_0 and T_1.

The numerical programs to calculate the reduced flow rates through capillaries and channels are available at the site: www.fisica.ufpr.br/sharipov. They may be inquired via the author too.

Table 3: Mass flow rate M through a capillary caused by the laser radiation vs height a and pressure P

P [Pa]	7.0	5.5	4.2	2.9	1.5
$M \times 10^{12}$ [mol/s]	2.6	2.0	1.5	0.96	0.48

3 LIGHT INDUCED DRIFT

The gas can be moved through a capillary by a laser beam. This phenomenon is called the light induced drift (LID). The effect is possible if an optically excitable gas has a transition frequency close to the laser frequency. Moreover, the cross section of the excited gaseous molecules must be different on that of the ground state particles. If the gas-surface accommodation coefficients also depend on the internal state of the particles the LID becomes stronger. The direction of the gas flow does not depend on the laser beam direction but it depends on the laser frequency.

The thermodynamic analysis of the phenomenon is given in the paper [5]. Some numerical calculations of the reduced flow rate can be found in the work [12]. The final expression of the reduced flow rate contains many characteristics of the laser radiation and of the gas. Some of them are unknown. That is why it is impossible to calculate the flow rate using these data.

For our estimation the experimental data [13] obtained for the gas CH_3F with the CO_2 laser can be used. The experiments were carried out with a quartz capillary having the radius a=0.75 mm and the length ℓ=300 mm. To realize the transition regime (Kn$\sim$1) the pressure of the gas was very low, about 4 ± 3 Pa.

Since the flow rate is very small it cannot be measured directly. The pressure difference on the capillary ends caused by the laser was measured. In stationary state the LID is compensated by the Poiseuille flow, which can be calculated via the pressure difference and the numerical data presented in [9]. In Table 3 the values of the flow rate M is given for different values of the pressure. One can see that the flow rate is almost proportional to the pressure.

The reciprocity relation of this phenomenon to the coupled one obtained in [5] can be used to find the optimum condition for the pumping of gas.

4 PHENOMENA IN MAGNETIC FIELD

As is known a polyatomic gas has anisotropic properties in the presence of magnetic field. As a consequence many new cross phenomena arise. For instance, the heat conductivity coefficient becomes a second order tensor, i.e. if the magnetic field has the z component, then a temperature gradient in the x direction causes the heat flux in the y direction. Below, two more examples of the cross phenomena in magnetic field are given.

4.1 Gyromagnetic effect

Consider a gas of polyatomic molecules confined between two coaxial cylinders in the presence of a magnetic field directed along the cylinder axis. If the cylinders have different temperatures, a torque appears between them. This effect was detected by Scott et al. [14]. The experiments were carried out for the internal cylinder with the radius 0.95 cm and with the length 20 cm. The outer cylinder was several times larger. The pressure was very low ($P = 6.65$ Pa) to reach the transition regime (Kn~1). The temperature difference $\Delta T = 50$ K between the gas and the internal cylinder was maintained. The torque on the internal cylinder reaches its maximum value for some given intensity of the magnetic field, which depends on the species of the gas. For instance, for the gases N_2 and O_2 the maximum value of the torque $\tau=0.022$ and 0.0065 dyn cm is reached at the intensity of the magnetic field $B=90$ and 3.5 Oe, respectively.

Till now there are no any reliable numerical data on the torque. To carry out such calculation the left hand side of the Boltzmann equation (3) must be modified taking into account the interaction of the gaseous molecules with the magnetic field.

In the paper [6] the conjugated cross phenomenon coupled with the gyromagnetic effect via the reciprocity relation is pointed out. The phenomenon is that: if the cylinders are maintained at the same temperature but one of them rotates a heat flux appears from one cylinder to the other.

4.2 Thermomagnetic effect

Let a channel joint two reservoirs containing a polyatomic gas. The horizontal plates of the channel are fixed at $y = \pm a/2$ and stretch over $-\ell/2 \leq x \leq \ell/2$ and $-b/2 \leq z \leq b/2$ as is shown in Fig.1. The vertical plates are fixed at $z = \pm b/2$. Let the magnetic field have the z component. In this case the temperature difference between the horizontal plates causes the gas flow in the x direction, i.e. the gas flows from one reservoir to the other. This phenomenon is called thermomagnetic effects. Changing the intensity of the magnetic field and/or the temperature difference one can control the flow rate through the channel.

There are no any numerical calculation of the effect to perform an estimation of the flow rate. To carry out these calculations the Boltzmann equation (3) must be applied.

In the paper [2] it was shown that in the same system the pressure difference between the reservoirs causes the heat flux between the horizontal plates. This phenomenon is coupled by the reciprocity relations to the thermomagnetic effect.
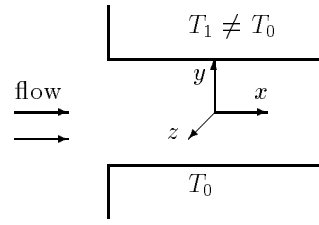

Figure 1: Sketch for the thermomagnetic effect

5 CONCLUSION REMARKS

The very few cross phenomena have been described in the present work. It is impossible in the frame of one paper to mention all cross phenomena that could be used in microfluidics. To select the most useful of them exact numerical solutions of the Boltzmann equation should be obtained for polyatomic gases interacting with a magnetic field or with a laser radiation. A close collaboration in this scientific field would very useful for both engineers designing microfluidics and specialists on the rarefied gas dynamics.

ACKNOWLEDGEMENT

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