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THE THERMOPHORESIS OF SOLIDS IN GASES†

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A brief review of existing ideas on the nature of the thermophoresis of solids in gases is given. A method for calculating the rate of thermophoresis of coarse solids is described. A procedure for analysing experimental data and for choosing a high-quality material on the basis of this is proposed. © 2005 Elsevier Ltd. All rights reserved.

1. INTRODUCTION

The kinetic theory of gases enables one, fairly simply, to calculate the rate of thermophoresis of a small body, which, as is assumed, slightly perturbs the state of the gas surrounding the body. The generally accepted formula for the rate of thermophoresis under so-called free-molecular conditions has the form [1, 2]

$$\mathbf{V}_{fm} = -\frac{3}{4}\frac{\eta}{\rho T_0}\frac{\operatorname{grad}T}{1+\pi\varepsilon/8} \tag{1.1}$$

where η is the dynamic viscosity, ρ is the density of the gas, ε is a coefficient characterizing the accommodation of momentum when gas molecules interact with the surface of the condensed phase, T_0 is the temperature at the centre of a spherical body, and $\operatorname{grad}T$ is the small constant temperature gradient far from the body. Some disagreement in the numerical factor in the denominator of formula (1.1) will be unimportant later.

The classical representation of the nature of thermophoresis of large bodies in gases is based on the discovery by Maxwell [3] and Reynolds [4] of the thermal slip of a gas along the interface. Epstein [5] made this the basis of the solution of the problem of the thermophoresis of large bodies as the boundary condition connecting the problem of the flow of a gas around a body and the problem of the temperature distribution, when a constant temperature gradient is maintained far from the body. Epstein's formula has the form

$$\mathbf{V}_{th}^{E} = -\frac{3}{4}\frac{\eta}{\rho T_0}\frac{\operatorname{grad}T}{1+\xi/2}, \quad \xi = \frac{\kappa_i}{\kappa} \tag{1.2}$$

where κ and κ_i are the thermal conductivities of the gas and of the condensed phase.

Epstein's paper gave an impetus to research on the nature of the thermophoresis of large bodies in gases. (When speaking of large bodies, we mean that the Knudsen number $\mathrm{Kn} = \lambda/R$, where λ is the mean free path of a gas molecule and R is a characteristic dimension of the body, is much less than unity.) Experiments subsequent to this showed that the mechanism of Maxwell slip does not exhaust all possible reasons for the phenomenon. In particular, this approach did not enable the experimentally observed unexpectedly high rate of thermophoresis of highly heat conducting bodies to be explained. Hence, a theoretical investigation of the problem has continued, and there is a considerable number of papers on this topic in the literature at the present time (see the reviews [6, 7]), in which various

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approaches and methods of calculation are employed. The results have turned out to be not completely identical. However, the general and undisputed conclusion is that the expression for the rate of thermophoresis of large bodies when $\mathrm{Kn} = 0$ has the form (1.2), apart from a numerical factor, which must be borne in mind when analysing any experimental and theoretical data on the thermophoresis of large bodies.

In the opinion of many researchers, a modified Epstein method gives the most satisfactory results. This is based on the solution of the problem which includes the Navier–Stokes and Fourier equations with boundary conditions which take slip into account. It is also more transparent physically. The paper by Waldmann and others [8] (see also [9]) turned out to be an important stage in the development of this method. In these papers, to obtain the boundary conditions, instead of using an heuristic approach, a method was proposed based on the use of the thermodynamics of irreversible processes. The boundary conditions in this case are obtained automatically. This approach immediately enabled all the discrepancies which arose previously when formulating the boundary conditions to be eliminated, and enabled them to be extended to the case of volatile bodies in gas mixtures.

We will briefly recall the procedure for calculating the rate of thermophoresis of large bodies in gases using the Epstein–Waldmann method.

2. FORMULATION OF THE PROBLEM

To solve the problem of the thermophoresis of large bodies we will consider the Stokes problem for a sphere around which a gas is flowing, at an infinite distance from which a small constant temperature gradient grad$T$ is maintained. We will confine ourselves to the case of non-volatile solids. This means formally that the surface of the sphere is impermeable for gas molecules, i.e. the normal component of the gas velocity at the body surface must be put equal to zero. (By considering the case of fairly large bodies, for which $\mathrm{Kn} \ll 1$, we can, by taking well-known precautions, drop certain terms proportional to Kn not only during the calculations but also at the stage of formulating the problem.) Hence, for the normal component of the velocity we have

$$v_r = 0 \tag{2.1}$$

The boundary condition for the tangential component of the gas velocity is less obvious. We will write it in the form [9]

$$v_\theta = \mathrm{Kn}\frac{R}{\eta}C_m\sigma_{r\theta} + k_{\mathrm{TS}}\frac{\eta}{\rho T_0}\frac{1}{R}\frac{\partial}{\partial\theta}\frac{T+T_i}{2} + \frac{3}{2}\frac{\eta}{\rho T_0}\frac{1}{R}\frac{\partial}{\partial\theta}\frac{T-T_i}{2} \tag{2.2}$$

The first two terms in expression (2.2) describe viscous and thermal slip. They are also contained in the Epstein model. Note, however, that we have made certain refinements here, namely: in the expression for the component of the viscous stress tensor $\sigma_{r\theta}$ we have taken into account, in addition to the usual stresses, also the thermal stress $\sigma_{r\theta}^{(T)}$, in the second term, instead of the numerical coefficient 3/4, the thermal slip coefficient k_{TS} is used. Moreover, we have written the expression for the tangential derivative of the temperature in more general form. However, the most important difference is the occurrence of the third term, which is not in the Epstein model.

We have used the following notation have: v is the gas velocity with respect to the body (the subscripts r and θ indicate the radial and tangential components respectively), C_m is the viscous slip coefficient, and T, T_i and T_0 are the temperature outside, inside and at the centre of the sphere respectively.

We will formulate the boundary conditions for determining the temperature in the Laplace problem. The normal component of the heat flux $\mathbf{q}$ at the boundary is continuous:

$$q_r = q_{ir}, \quad \text{or} \quad \partial T/\partial r = \xi \partial T_i/\partial r \tag{2.3}$$

For the temperature we have (this is essentially the Smoluchowski relation [10] in improved form)

$$T - T_i = \mathrm{Kn}\kappa^{-1}C_t(\mathbf{q} + \mathbf{q}_i)_r/2 \tag{2.4}$$

where C_t is the temperature jump coefficient.

3. THE DISTRIBUTION OF THE GAS VELOCITY AND THE TEMPERATURE

Expressions for the components of the gas velocity in the neighbourhood of the body and for the force with which the gas acts on the body, can be written in the following standard form

$$v_r = v_0\left[1-2a\frac{R}{r}+2b\left(\frac{R}{r}\right)^3\right]\cos\theta,\quad v_\theta = -v_0\left[1-a\frac{R}{r}-b\left(\frac{R}{r}\right)^3\right]\sin\theta;\quad \mathbf{F} = 8\pi\eta Ra\mathbf{v}_0$$

where $\mathbf{v}_0$ is the free-stream velocity of gas. In equilibrium, taking the boundary condition (2.1) into account, we have for the constants of integration: $a = 0$ and $b = -1/2$.

We will write the temperature distributions inside and outside the body in the form

$$T_i = T_0+(\mathbf{Ar}),\quad T = T_0+(\mathrm{grad}T\mathbf{r})+(\mathbf{Br})(R/r)^3 \tag{3.1}$$

From conditions (2.3) and (2.4) we have

$$-2\mathbf{B}+\mathrm{grad}T = \xi\mathbf{A},\quad \mathbf{B}+\mathrm{grad}T-\mathbf{A} = C_t\mathbf{A}\xi\mathrm{Kn}/2$$

Hence we obtain

$$\mathbf{A} = \frac{3}{2}\frac{1}{1+\xi/2}\mathrm{grad}T,\quad \mathbf{B} = \frac{1}{2}\frac{1-\xi}{1+\xi/2}\mathrm{grad}T \tag{3.2}$$

Finally, we have for the thermal stress in the gas

$$\sigma_{r\theta}^{(T)} = \frac{3}{r}\frac{\eta^2}{\rho T_0}\left[\frac{1}{r}-\frac{\partial}{\partial r}\right]\frac{\partial T}{\partial\theta} = -\frac{9}{2R}\frac{\eta^2}{\rho T_0}\frac{1-\xi}{1+\xi/2}\sin\theta\,\mathrm{grad}T \tag{3.3}$$

4. RATE OF THERMOPHORESIS

Using Eq. (2.2) and bearing in mind that the equilibrium velocity of the body (the rate of thermophoresis) is equal to the equilibrium value v_0, taken with the opposite sign, we have

$$\mathbf{V}_{\mathrm{th}} = -k_{\mathrm{TS}}\frac{\eta}{\rho T_0}\frac{\mathrm{grad}T}{1+\xi/2}\left\{1+\xi\mathrm{Kn}\left[\frac{1}{2}C_t+\frac{3}{k_{\mathrm{TS}}}\left(\frac{1}{4}C_t-C_m\right)\right]\right\} \tag{4.1}$$

We recall that, as a result of using the condition that the Knudsen number is small, we have dropped a number of terms, including also in expression (4.1). We must, however, emphasise that a situation is possible when the thermal conductivity of the body is so high that even for small Knudsen numbers $\xi\mathrm{Kn} \gg 1$ (this situation occurs, for example, for metal bodies). Hence, terms containing the factor $\xi\mathrm{Kn}$ are retained. If the thermal conductivity of the body is not too high compared with the thermal conductivity of the gas, the second term in braces in expression (4.1) is also small compared with unity and can be neglected, which leads to the refined Epstein formula (1.2).

Relation (4.1) can be written in the form of the following expression for the reduced rate of thermophoresis in a continuous medium

$$\begin{aligned} V_{\mathrm{thr}} &= -\frac{\mathbf{V}_{\mathrm{th}}T_0(1+\xi/2)}{\eta\rho^{-1}\mathrm{grad}T} = k_{\mathrm{TS}}(\varepsilon)(1+\xi\mathrm{Kn}\Delta(\varepsilon,\alpha)) \\ \Delta(\varepsilon,\alpha) &= \frac{1}{2}\left[C_t(\alpha)+\frac{3}{k_{\mathrm{TS}}(\varepsilon)}\left(\frac{1}{2}C_t(\alpha)-2C_m(\varepsilon)\right)\right] \end{aligned} \tag{4.2}$$

We will also give an expression for the reduced rate of thermophoresis in the free-molecule limit

$$V_{\mathrm{fmr}} = -\frac{\mathbf{V}_{\mathrm{fm}}T_0}{\eta\rho^{-1}\mathrm{grad}T} = \frac{3}{4}\frac{1}{1+\pi\varepsilon/8} \tag{4.3}$$

Table 1

α	$\varepsilon = 0.1$	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
0.1	−18.1	16.6	26.8	3.2	33.4	34.5	35.2	35.5	35.6	35.6
0.2	−43.5	−7.76	3.47	8.59	11.4	13.1	14.2	14.9	15.4	15.8
0.3	−51.9	−15.8	−4.33	1.04	4.05	5.92	7.16	8.03	8.65	9.11
0.4	−56.2	−19.8	−8.25	−2.76	0.36	2.32	3.64	4.57	5.26	5.77
0.5	−58.8	−22.3	−10.6	−5.05	−1.87	0.14	1.51	2.48	3.21	3.75
0.6	−60.5	−23.9	−12.2	−6.59	−3.37	−1.32	0.08	1.08	1.83	2.40
0.7	−61.7	−25.1	−13.3	−7.70	−4.45	−2.37	−0.95	0.07	0.83	1.42
0.8	−62.7	−26.0	−14.2	−8.54	−5.27	−3.17	−1.73	−0.70	0.08	0.68
0.9	−63.4	−26.7	−14.9	−9.21	−5.92	−3.80	−2.35	−1.30	−0.51	0.10
1	−64.1	−27.3	−15.5	−9.75	−6.44	−4.31	−2.85	−1.79	−0.99	−0.38

To calculate the kinetic coefficients occurring in (4.1), we will use the results of a calculation obtained from the data given in [11] for the solid-sphere model

ε	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
k_{TS}	0.81	0.87	0.93	0.98	1.02	1.07	1.11	1.15	1.18	1.22
C_m	18.20	8.78	5.62	4.03	3.07	2.42	1.95	1.60	1.32	1.09

and the formula [12]

$$C_t(\alpha) = 1.78(2/\alpha - 1)(1 + 0.162\alpha)$$

Here α is a coefficient representing the energy accommodation when gas molecules interact with the surface of the condensed phase.

The values of $\Delta(\varepsilon, \alpha)$ obtained are given in Table 1.

Table 1 enables us, by specifying the ratio of the thermal conductivities of the body and the gas ξ, to calculate from formula (4.2) the rate of thermophoresis of bodies with $\mathrm{Kn} \ll 1$ as a function of the Knudsen number over the whole range of values of α and ε from 0.1 to 1. In principle, any possible curve of $V_{\mathrm{thr}}(\mathrm{Kn})$ when $\mathrm{Kn} \ll 1$ must lie inside the region bounded by the two rays. For example, if we confine ourselves to the range of values of α and ε from 0.8 to 1, the curve of the reduced rate of thermophoresis V_{thr} against the Knudsen number must intersect the ordinate axis at a point with ordinate lying between the values 1.15 and 1.22, and its slope, defined by the function $\Delta(\alpha, \varepsilon)$ must lie between the values $0.68\,\xi$ and $-1.79\,\xi$ (Fig. 1). The experimental points obtained by Kanki and Iuchi [13], do not satisfy either of these conditions and must be rejected. The same can be said of the results of measurements for $\xi = 0.8$ [13] (Fig. 1), and also for $\xi = 0.3$ [14, 15], presented in Fig. 2. Only the data for $\xi = 8.13$ [16] (Fig. 3) show good agreement with the predictions of the model: the experimental points lie on the calculated curve $\varepsilon = 1$, $\alpha = 0.92$, which correlates excellently with existing ideas and the results of other measurements. In all the figures the continuous semi-bold straight line corresponds to the calculated straight line for values of $\varepsilon = 0.8$ and $\alpha = 1$, while the dashed line is for $\varepsilon = 1$ and $\alpha = 0.8$; the arrows on the right indicate the corresponding values of V_{fmr}. The dash-dot lines are linear approximations of the experimental data obtained by the method of least squares.

Unfortunately, since data of other experiments in the region $\mathrm{Kn} \ll 1$ is not available, it is not possible to analyse them.

5. DISCUSSION OF THE RESULTS

During the last few years an estimate of the experimental data by comparing them with the interpolation formula derived by Talbot *et al.* [17] has become widely used. It is obvious, however, that this interpolation, at least when $\mathrm{Kn} \ll 1$, where it is based on the clearly unsatisfactory Brock formula [18], is unconvincing. A more important consideration is the fact that the existing experimental methods of measuring the rate of thermophoresis give a quite considerable spread of data, so that such a comparison may in the best case only indicate qualitative agreement between the model [17] and experiment. (This also applies, incidentally, to a comparison of experimental results even with the most reliable theoretical

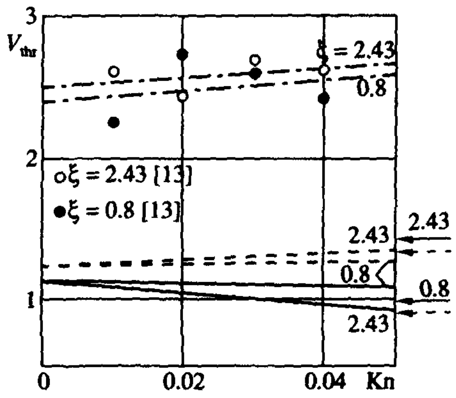

Fig. 1

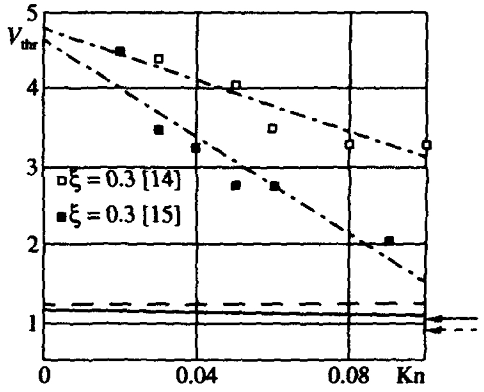

Fig. 2

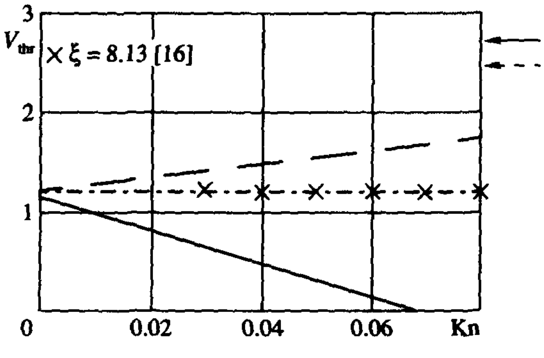

Fig. 3

data, for example [19].) Nevertheless, may researches assert that the experimental data they have obtained agree completely with the theoretical data. The method proposed in this paper for estimating the results of measurements (and even of the procedures themselves) enables one to make a selection uniquely and practically independently of their accuracy, i.e. to discard unsatisfactory experimental data, thereby retaining essentially admissible data. When the criteria of reliability are satisfied, the possibility is opened up of fairly accurately estimating the values of the energy accommodation coefficients and the momentum when gas molecules collide with the surface of the body (the aerosol particle) by fitting the theoretical and experimental curves.

REFERENCES

1. BAKANOV, S. P. and DERYAGIN, B. V., The theory of the thermoprecipitation of highly dispersed aerosol systems. *Kolloid. Zh.*, 1959, **21**, 4, 377–384.
2. WALDMANN, L., Über die Kfraft eines inhomogenen Gases auf kleine suspendierte Kugeln. *Z. Naturforsch.*, 1959, **14a**, 7, 589–599.
3. MAXWELL, J. C., On stresses in rarefied gases arising from inequalities of temperature. *Phil. Trans. Royal Soc. of London.*, 1879, **170**, Pt 1, 231–256.
4. REINOLDS, O., On certain dimensional properties of matter in the gaseous state. *Phil. Trans. Roy. Soc. Ser.B.*, 1880, **170**, 727–845.
5. EPSTEIN, P. S., Zur theorie des Radiometers. *Z. Physik*, 1929, **54**, 7/8, 537–563.
6. BAKANOV, S. P., Thermophoresis in gases at small Knudse numbers. *Aerosol Sci. Technol.*, 1991, **15**, 2, 77–92.
7. BAKANOV, S. P., Thermophoresis in gases at small Knudsen numbers. *Usp. Fiz. Nauk*, 1992, **162**, 9, 133–152.
8. WALDMANN, L., Non-equilibrium thermodynamics of boundary conditions. *Z. Naturforsch.*, 1967, **22a**, 8, 1269–1280.
9. BAKANOV, S. P. and ROLDUGIN, V. I., Boundary-value problems of the kinetic theory of gases and irreversible thermodynamics. *Prikl. Mat. Mekh.* 1977, **41**, 4, 651–659.
10. SMOLUCHOWSKI, M., Über den Temperatursprung bei Wärmeleitung in Gasen. *Sitzber. Akad. Wiss. Wien*, 1898, **107**, 304–329.
11. BAKANOV, S. P., Calculation of thermal slip for arbitrary accommodation of a gas at the interface. *Zh. Tekh. Fiz.*, 1977, **47**, 2, 421–427.
12. ONISHI, Y., Effect of accommodation coefficient on thermal creep flow of rarefied gas. *Trans. Japan. Soc. Aeronaut and Space Sci.*, 1972, **15**, 29, 117–123.
13. KANKI, T. and IUCHI, S., Accurate measurements of thermal and diffusion forces on a spherical particle. *Rarefied Gas Dynamics: Proc. 14th Intern. Symp.* Univ. Tokyo Press, Tokyo, 1984, 865–872
14. DAVIS, L. A. and ADAIR, T. W. III., Thermal force on a sphere. *J. Che. Phys.*, 1975, **62**, 6, 2278–2285.
15. TONG, N. T., Experiments on photophoresis and thermophoresis. *J. Colloid Interface Sci.*, 1975, **51**, 1, 143–151.
16. ROSENBLATT, P. and LAMER, V. K., Motion of a particle in a temperature gradient. *Phy. Rev.*, 1946, **70**, 5/6, 385–395.
17. TALBOT, L., CHENG, R. K., SCHEFFER, R. W. and WILLIS, D. R., Thermophoresis of particles in a heated boundary layer. *J. Fluid Mech.*, 1980, **101**, Pt 4, 737–758.
18. BROCK, J. R., Comments on "Thirteen-Moment Theory of the Thermal Force on a Spherical Particle." *Phys. Fluids*, 1968, **11**, 4, 922–933.
19. SONE, Y. and AOKI, K., Negative thermophoresis: thermal stress slip flow around a spherical particle in a rarefied gas. *Progress in Astronautics and Aeronautics*, AIAA, New York, 1981, **74**, Pt 1, 849–503.

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