

# HEAT TRANSFER AND TEMPERATURE JUMP IN A POLYATOMIC GAS\*

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**Abstract**—A variational principle based on the integro-differential form of the linearised Wang Chang-Uhlenbeck equation, with general boundary conditions, is used to evaluate the heat conducted through a polyatomic gas between parallel plates. The result is an accurate, closed form expression for the heat transfer, valid for all degrees of rarefaction, rational in the inverse Knudsen number, and parametrised by the thermal accommodation coefficients, the heat capacity of the internal modes, full range moments of the Chapman-Enskog solution and half range bracket integrals of the free molecular solution. The temperature jump coefficient is obtained from the high density expansion of the heat flux and is dependent on the thermal accommodation coefficients, the internal heat capacity, and moments of the Chapman-Enskog solution. In the limit of vanishing internal specific heat, both the heat transfer and the temperature jump reduce to results previously given for the monatomic gas.

## NOMENCLATURE

|                            |  |                            |   |
|----------------------------|--|----------------------------|---|
| $A, A_{j \rightarrow i}$ , | linearized boundary operator and boundary kernel respectively equation (11); | $F$ ,                      | Eucken factor $F = m\lambda/\mu c_v$ ;                    |
| $a_i(c)$ ,                 | Chapman Enskog heat conductivity solution;                                   | $\tilde{g}$ ,              | dimensional relative velocity;                            |
| $B_{j \rightarrow i}$ ,    | kernel of the general boundary conditions equation (2);                      | $h$ ,                      | perturbation of the distribution;                         |
| $c$ ,                      | dimensionless molecular velocity $c = \xi(2\mathcal{R}T_0)^{-1/2}$ ;         | $\gamma_{ij}^{kl}$ ,       | dimensional scattering cross section;                     |
| $c_v^i$ ,                  | internal specific heat per molecule;   | $k$ ,                      | Boltzmann constant;                                       |
| $c_v$ ,                    | total specific heat $c_v = \frac{3}{2}k + c_v^i$ ;                           | $l$ ,                      | mean free path;   |
| $E_i$ ,                    | internal energy of level $i$ (dimensional);                                  | $M_{w_i}$ ,                | Maxwell-Boltzmann distribution at the wall temperature;   |
| $f_i$ ,                    | molecular velocity distribution for particles in level $i$ ;                 | $m$ ,                      | molecular mass;   |
| $f_{0i}$ ,                 | absolute Maxwell-Boltzmann distribution;                                     | $N_0$ ,                    | number density at $x = 0$ ;                               |
|                            |  | $p_0$ ,                    | gas pressure at $x = 0$ , $p_0 = N_0 k T_0$ ;             |
|                            |  | $\mathcal{R}$ ,            | gas constant;   |
|                            |  | $R$ ,                      | reflection operator;                                      |
|                            |  | $Q$ ,                      | partition function  |
|                            |  | $Q = \sum \exp(-E_j/kT)$ ; |   |
|                            |  | $\tilde{Q}_{T,x}$ ,        | total heat transfer in $x$ direction (dimensional);       |
|                            |  | $T_w, T_0$ ,               | wall temperature and temperature at $x = 0$ respectively; |
|                            |  | $u_0$ ,                    | wall velocity;  |
|                            |  | $v$ ,                      | peculiar velocity;  |
|                            |  | $\tilde{x}$ ,              | spatial coordinate;                                       |
|                            |  | $x$ ,                      | dimensionless coordinate perpendicular to the plates;     |

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| $z_c$ ,                                    | collisional relaxation number;   |
| $\alpha_{tr}, \alpha_{int}$ ,              | thermal accommodation coefficients for translational and internal energy respectively; |
| $\beta_i (i=1, 2, 3)$ ,                    | variational constants;   |
| $\gamma$ ,                                 | ratio of specific heats;   |
| $\delta$ ,                                 | plate separation (dimensional);  |
| $\delta$ ,                                 | inverse Knudsen number $\delta = \delta/l$ ;   |
| $\varepsilon_i$ ,                          | dimensionless internal energy<br>$\varepsilon_i = E_i/kT_0$ ;                          |
| $\theta$ ,                                 | collisional scattering angle;  |
| $\lambda_T, \lambda_{tr}, \lambda_{int}$ , | thermal conductivities;  |
| $\mu$ ,                                    | gas viscosity;   |
| $\xi$ ,                                    | molecular velocity (dimensional);  |
| $\rho_0$ ,                                 | $mN_0$ ;   |
| $\tau$ ,                                   | temperature perturbation<br>$\tau =  (T_w - T)/T_0 $ ;                                 |
| $\tau_R$ ,                                 | relaxation time for the internal degrees of freedom;                                   |
| $\tau_c$ ,                                 | inverse of the total collision frequency;  |
| $\omega$ ,                                 | solid angle of scattering;   |
| $\mathcal{E}$ ,                            | temperature jump coefficient.  |

### INTRODUCTION

ALTHOUGH the kinetic theory of plane heat conduction has been exhaustively treated for a monatomic gas [1-5], the corresponding problem for a polyatomic gas has received considerably less attention due to the complexity of the molecular collision process and of the molecule-wall interaction. Most work on the polyatomic problem has been concerned with the calculation of transport coefficients using the Chapman-Enskog procedure on a suitable kinetic equation [6, 7]. A notable exception to this is the work of Hsu and Morse [8-10] who have treated the full boundary value problem with a generalization of Maxwell's boundary condition and with suitable models of the collision term of the Wang Chang-Uhlenbeck equation [11, 12]. The extent of numerical computation necessary to achieve quantitative results is discouraging.

In light of recent work on the monatomic problem [5], it seems that many of the more cumbersome aspects of the problem may be eliminated through the use of appropriate variational techniques. In fact great generality can be obtained from the outset, since there need be no restriction to the form of the collision operator and the boundary conditions used can be quite general. In particular, with a variational technique based on the integrodifferential form of the equation, the heat transfer may be found in a closed form which reduces to all known limits correctly [5]. Thus it appears that a recalculation of the polyatomic heat transfer could be useful.

In the following the boundary value problem is formulated for the linearised Wang Chang-Uhlenbeck equation [13] with general boundary conditions and certain formal similarities with the corresponding monatomic formulation are noted. By exploiting these similarities, the solution of the general problem can be shown to be equivalent to making a certain quadratic functional stationary. For the heat transfer problem treated here, the stationary value of this functional is related to heat transfer to the boundary and can be approximately evaluated with great accuracy by using an appropriate trial function. Explicit expressions are given for the heat transfer and the temperature jump coefficient which agree with the monatomic results previously given in the limit of vanishing internal specific heat. Furthermore, the expression for the heat transfer reproduces correctly the free molecular, near free molecular and continuum results that are obtained from the linearised equation.

### BASIC EQUATIONS AND FORMULATION

In this section the full boundary value problem for the linearised Wang Chang-Uhlenbeck equation is formulated with general boundary conditions. A dilute gas of spherically symmetric polyatomic molecules is considered in some region  $\Omega$  of physical space bounded by the

surface  $\partial\Omega$ . The molecules are treated semi-quantum mechanically in the sense that the internal energy of the particles is quantized but the translational energy is treated classically. To each internal quantum state, with internal energy  $E_i$ , is assigned a velocity distribution function  $f_i$ . The energy  $E_i$  is a parameter which completely specifies the internal state in this approximation. The spatial and temporal evolution of  $f_i$  due to collisions is given by [13]

$$\frac{\partial}{\partial t} f_i + \xi \frac{\partial}{\partial \bar{x}} f_i = \sum_{jkl} [f_k f_l - f_i f_{j_s}] \tilde{g} \tilde{I}_{ij}^{kl}(\tilde{g}, \theta) d\omega d\xi_s \quad \bar{x} \in \Omega \quad (1)$$

where tildes denote dimensional quantities and, in standard notation,  $\tilde{g}$  is the relative velocity before collision,  $\tilde{I}_{ij}^{kl}$  is the collision cross section, which depends only on  $\tilde{g}$  and the scattering angle  $\theta = \tilde{g} \cdot \tilde{g}' / \tilde{g} \tilde{g}'$  due to the symmetry of the molecules, and  $f_{i_s}$  denotes  $f_i(\xi'_s)$  where primes indicate post-collisional quantities. This form of the equation, due to Wang Chang, Uhlenbeck and de Boer [13], follows from microscopic reversibility of the collisions due to time reversal invariance of quantum mechanics in the absence of degeneracy. This has been discussed in detail by Waldmann [14, 15].

The boundary conditions to be matched to equation (1) can be written as [16, 17]

$$|(\xi - u_0) \cdot n| f_i(\bar{x}_0, \xi) = \sum_{(\xi' - u_0) \cdot n < 0} \int B_{j \rightarrow i}(\xi' \rightarrow \xi) f_j(\bar{x}_0, \xi') |(\xi' - u_0) \cdot n| d\xi' : \quad \bar{x}_0 \in \partial\Omega, \quad (\xi - u_0) \cdot n > 0 \quad (2)$$

where  $u_0$  denotes the wall velocity at  $\bar{x}_0$  and  $n$  is the normal pointing into the gas. For a non-porous wall, the positive kernel  $B_{j \rightarrow i}$  (assumed to be independent of the state of the gas) is normalized:

$$\sum_i \int_{(\xi' - u_0) \cdot n > 0} B_{j \rightarrow i}(\xi' \rightarrow \xi) d\xi = 1 : \quad \bar{x}_0 \in \partial\Omega, \quad (\xi' - u_0) \cdot n < 0 \quad (3)$$

thus we may write  $(\xi - u_0) \cdot n = v \cdot n$  where  $v$  is the peculiar velocity of the gas as at the wall.

The reciprocity of  $B_{j \rightarrow i}$  is written as

$$|v' \cdot n| M_{w_j}(\xi') B_{j \rightarrow i}(\xi' \rightarrow \xi) = |v \cdot n| M_{w_i}(\xi) B_{i \rightarrow j}(-\xi \rightarrow -\xi') : \quad \bar{x}_0 \in \partial\Omega; \quad v \cdot n > 0; \quad v' \cdot n < 0 \quad (4)$$

and follows also from the time reversal invariance of quantum mechanics in the absence of degeneracy, as discussed by Kušćer [18]. A consequence of reciprocity and non-porosity is that the velocity distribution of a gas in equilibrium with the wall is unchanged by collisions with the wall. Thus,

$$|v \cdot n| M_{w_i}(\xi) = \sum_{j \neq i} \int_{v' \cdot n < 0} B_{j \rightarrow i}(\xi' \rightarrow \xi) |v' \cdot n| M_{w_j}(\xi') d\xi' : \quad \bar{x}_0 \in \partial\Omega; \quad v \cdot n > 0 \quad (5)$$

where

$$M_{w_i}(\xi) = N_w (2\pi \mathcal{R} T_w)^{-\frac{3}{2}} Q_w^{-1} \exp \left[ -\frac{mv^2}{2kT_w} - \frac{E_i}{kT_w} \right]; \quad Q_w = \sum_s \exp \left[ -\frac{E_s}{kT_w} \right] \quad (6)$$

is a Maxwell-Boltzmann distribution with the temperature and velocity of the wall.

The kernel  $B_{j \rightarrow i}(\xi' \rightarrow \xi)$  must be specified by the details of the wall interaction at the molecular level. In the absence of a rigorous theory, various specialized assumptions are made; the most common being Maxwell's assumption of partial diffuse and specular reflection. When extended to allow for internal degrees of freedom  $B_{j \rightarrow i}^{\max}$  becomes

$$B_{j \rightarrow i}^{\max} = \alpha_{\text{int}} \alpha_n + N_w Q_w^{-1} (2\pi \mathcal{R} T_w)^{-\frac{3}{2}} \exp \left[ -\frac{v^2}{2\mathcal{R} T_w} - \frac{E_i}{kT_w} \right] |v \cdot n| + (1 - \alpha_{\text{int}}) \alpha_n + \delta_{ij} N_w (2\pi \mathcal{R} T_w)^{-\frac{3}{2}} \times \exp \left[ -\frac{v^2}{2\mathcal{R} T_w} \right] |v \cdot n| + (1 - \alpha_n +) \alpha_{\text{int}} \delta [ \xi' - \xi + 2m(n \cdot v) ] \times Q_w^{-1} \exp \left[ -\frac{E_i}{kT_w} \right]$$

$$+ (1 - \alpha_{n+})(1 - \alpha_{int}) \delta_{ij} \delta[\xi' - \xi + 2\mathbf{n} \cdot \mathbf{v}] \quad (7)$$

where  $N_w$  is fixed by the normalization as  $(2\pi/\mathcal{R}T_w)^{3/2}$ , and  $\alpha_{int}$  and  $\alpha_{n+}$  are the thermal accommodation coefficients for the internal and translational energy respectively.

If the distribution  $f_i$  can be considered to be a small deviation from some basic Maxwell-Boltzmann distribution  $f_{0i}$ , we may write

$$f_i = f_{0i}(1 + h_i) \quad \|h_i\| \ll 1 \quad (8)$$

where

$$f_{0i} = N_0(2\pi \mathcal{R}T_0)^{-3/2} Q_0^{-1} e^{-c^2/\varepsilon_i}; \quad c^2 = \frac{\xi^2}{2\mathcal{R}T_0},$$

$$\varepsilon_i = \frac{E_i}{kT_0}, \quad Q_0 = \sum_s e^{-\varepsilon_s} \quad (9)$$

and the constants  $N_0$  and  $T_0$  represent some appropriately chosen density and temperature of the gas. With this linearization we have

$$\xi \cdot \frac{\partial h}{\partial \bar{\mathbf{x}}} = N_0 L h \quad \bar{\mathbf{x}} \varepsilon \Omega$$

$$L h = \sum_{jkl} \frac{\exp(-c_s^2 - \varepsilon_j)}{Q_0 \pi^{3/2}} [h'_k + h'_{l_s} - h_i - h_{j_s}] \quad \bar{g} I_{ij}^{kl}(g, \theta) d\omega dc_s \quad (10)$$

with the boundary conditions

$$h_i^+ = h_0 + A h^- \quad \mathbf{v} \cdot \mathbf{n} > 0 \quad \bar{\mathbf{x}}_0 \varepsilon \partial \Omega$$

$$A h^- = \sum_j \int_{\mathbf{v}' \cdot \mathbf{n} < 0} A_{j \rightarrow i}(\xi' \rightarrow \xi) h_j(\xi') d\xi' \quad \mathbf{v} \cdot \mathbf{n} > 0$$

$$A_{j \rightarrow i} = [|\mathbf{v} \cdot \mathbf{n}| f_{0i}(\xi)]^{-1} B_{j \rightarrow i}(\xi' \rightarrow \xi) |\mathbf{v}' \cdot \mathbf{n}| f_{0j}(\xi') \quad (11)$$

and  $h_{0i}$  is the known source term

$$h_{0i} = \sum_j \int_{\mathbf{v}' \cdot \mathbf{n} < 0} A_{j \rightarrow i}(\xi' \rightarrow \xi) d\xi' - 1. \quad (12)$$

By linearizing the kernel  $A_{j \rightarrow i}$  in the small parameters  $[(T_w - T_0)/T_0]$  and  $\mathbf{u}_w$ , the kernel  $A_{j \rightarrow i}$  depends only on the parameters of the basic

distribution  $f_{0i}$ . As a result, the inhomogeneous term can be written as

$$h_{0i}^+ = \psi_{0i}^+ - A \psi_{0i}^-$$

$$\psi_{0i} = \frac{T_w - T_0}{T_0} (c^2 - \frac{3}{2} + \varepsilon_i - \frac{c_v^i}{k}) + \frac{1}{\mathcal{R}T_0} \mathbf{u}_w \cdot \mathbf{v} \quad (13)$$

where  $c_v^i$  is the internal specific heat of the gas

$$\frac{c_v^i}{k} = Q_0^{-1} \sum_i \varepsilon_i e^{-\varepsilon_i}.$$

It is noted here that the introduction of the internal degrees of freedom in this spherically symmetric, non-degenerate approximation has little effect on the formulation as compared to the monatomic problem. The principal differences are that now the total energy is a collision invariant

$$L(c^2 + \varepsilon_i) = 0 \quad (14)$$

and the inhomogeneous boundary term now contains a term proportional to the internal energy.

#### THE VARIATIONAL PRINCIPLE

Recently a variational principle has been used in conjunction with the integrodifferential form of the linearized Boltzmann equation and general boundary conditions which is capable of giving extremely accurate results for certain macroscopic quantities of physical interest [5, 19]. This technique has the further advantage of being extremely easy to apply and gives simple, closed form results for the quantity in question valid throughout the transition regime. The principal disadvantage seems to be that the technique is limited to problems in which the adjoint equation and adjoint boundary conditions are simply related to the direct equation and direct boundary conditions. This latter restriction can be removed, however, by considering the method of Roussopolous [20-22]. In the heat transfer problem to be considered here the two methods are identical.

The extension of this technique to the polyatomic problem formulated in the preceding section is quite direct. In particular, with the following inner products defined:

$$(f, g) = \sum_i \int d\mathbf{c} \frac{e^{-c^2 - \epsilon_i}}{Q_0 \pi^{\frac{3}{2}}} f_i(\mathbf{c}) g_i(\mathbf{c}); [f, g] = \int_{\Omega} d\mathbf{x} (f, g) \quad (15)$$

$$(f, g)_B = \sum_{i, c, n > 0} \int d\mathbf{c} \frac{e^{-c^2 - \epsilon_i}}{Q_0 \pi^{\frac{3}{2}}} |c \cdot \mathbf{n}| f_i(\mathbf{c}) g_i(\mathbf{c});$$

$$[f, g]_B = \int_{\partial\Omega} ds (f, g)_B \quad (16)$$

we have, for arbitrary functions  $f(\mathbf{x}, \mathbf{c})$  and  $g(\mathbf{x}, \mathbf{c})$ :

$$[R(D - L)f, g] = [f, R(D - L)g] + [g^+, Rf^-]_B - [Rg^-, f^+]_B \quad (17)$$

$$[ARf, g]_B = [f, ARg]_B \quad (18)$$

where  $R$  is the reflection operator

$$Rf(\mathbf{x}, \mathbf{c}) = f(\mathbf{x}, -\mathbf{c}) \quad (19)$$

and  $D = \mathbf{c} \cdot (\partial/\partial\mathbf{x})$ . In arriving at equation (17), use was made of the self-adjointness of  $L$  in the inner product (15) due to the relation [15]

$$g^2 \tilde{I}_{ij}^{kl}(\mathbf{g}, \theta) = g'^2 \tilde{I}_{ki}^{lj}(\mathbf{g}', \theta) \quad (20)$$

and the rotational invariance of  $L$ , which follows from the assumption of spherical symmetry of the particles. Equation (18) follows directly from reciprocity of the boundary operator and is analogous to the result given by Cercignani [16, 17]. The boundary terms on the right hand side of equation (15) appear because  $f$  and  $g$  do not in general satisfy the boundary conditions. The utility of these relations is that the functional  $J(\tilde{h})$  defined as

$$J(\tilde{h}) = [R(D - L)\tilde{h}, \tilde{h}] + [\tilde{h}^+ - A\tilde{h}^- - 2h_0, R\tilde{h}^-]_B \quad (21)$$

has the variation  $\delta J$  given by

$$\delta J = 2[R(D - L)\tilde{h}, \delta\tilde{h}] + 2[\tilde{h}^+ - A\tilde{h}^- - h_0, R\delta\tilde{h}^-]_B \quad (22)$$

Thus solving (10) with the boundary conditions (11) is equivalent to making  $J(\tilde{h})$  stationary. Furthermore the stationary value attained by  $J$  when  $\tilde{h} = h$  has been shown to be related to certain quantities of physical interest [19]. The practical use of such a result is that the stationary condition

$$\delta J = 0 \quad (23)$$

can be used to obtain a "best fit" of adjustable parameters in a suitable trial function such that the stationary value of  $J$ , and thus the macroscopic quantities associated with it, can be accurately predicted. Since the inhomogeneous term of equation (13) differs from the monatomic case only in the addition of the internal energy, it is clear from [19] that the stationary value of  $J$  in this case is related to the total heat transfer to the body.

#### APPLICATION TO PLANE HEAT TRANSFER

The problem of polyatomic heat transfer between parallel plates has been previously treated by means of a half-range moment method [8] and later using a variational technique in conjunction with a suitable kinetic model for the polyatomic collision process [9, 10]. This latter work includes a complete numerical study of the boundary value problem including temperature and density profiles as well as a parametric study of the relaxation properties of the gas and a good comparison of the calculated heat transfer with experiment [23]. Good agreement is found for the heat transfer but the density, which is not related to the stationary value of the functional used, is less well described. It is the purpose of the present work to present an analytically manageable result for the total heat transfer which accurately describes the transition regime in an attempt to overcome some the inherent numerical complications of the previous formulations. Detailed numerical evaluation and comparison with experiment will not be presented here.

We consider two parallel, stationary plates

in the planes  $x = \pm \delta/2$  with the temperatures  $T_w^\pm = T_0(1 \mp \tau)$ ;  $\tau = \Delta T/T_0 \ll 1$ . Neglecting all variations in the directions parallel to the plates leads to the one dimensional equations:

$$c_x \frac{\partial h}{\partial x} = Lh \quad x \in \left[ -\frac{\delta}{2}, \frac{\delta}{2} \right] \quad (24)$$

$$h^+ = h_0 + Ah^- \quad x = -\frac{\delta}{2} \operatorname{sgn} c_x \quad (25)$$

where  $\operatorname{sgn}(\pm x^2) = \pm 1$  and distance is measured in units of the mean free path  $l$  and  $\delta$  is to be interpreted as an inverse Knudsen number based on  $l$  and the dimensional plate separation. In the collision term  $L$ ,  $\bar{g}I_{ij}^k$  is non-dimensionalized by  $N_0 l (2RT_0)^{-\frac{1}{2}}$ . The constants  $N_0$  and  $T_0$  are chosen to be the density and temperature of the gas at  $x = 0$ , and, in this antisymmetrical problem, represent the average density and temperature.

Although the condition on the perturbed distribution at the plates is generally given by the linearized version of equation (7), in this work a slightly different method of introducing thermal accommodation coefficients is used, based on a recent formulation due to Cercignani and co-workers [3, 24]. The effects of the different forms of the boundary conditions have been shown to be slight and probably not experimentally detectable in the heat transfer [5]. In this formulation it is assumed that the perturbed distribution emitted from the wall may be written as

$$h_i^+ = \gamma^* + \tau_{tr}^*(c^2 - 2) + \tau_{int}^* \left( \varepsilon_i - \frac{c_v^i}{k} \right) \quad (26)$$

$$x = -\frac{\delta}{2} \operatorname{sgn} c_x$$

The coefficients are determined by the conservation of mass at the solid boundary and by the definitions of the accommodation coefficients:

$$\begin{aligned} |\mathbf{n} \cdot \mathbf{u}^{in}| &= |\mathbf{n} \cdot \mathbf{u}^{out}| \\ (1 - \alpha_{tr}) \bar{Q}_{tr}^{in} &= \bar{Q}_{tr}^{out} - \alpha_{tr} \bar{Q}_{tr}^w \\ (1 - \alpha_{int}) \bar{Q}_{int}^{in} &= \bar{Q}_{int}^{out} - \alpha_{int} \bar{Q}_{int}^w \end{aligned} \quad (27)$$

Here  $\mathbf{u}^{in}$  is the velocity of the stream approaching the wall,  $\bar{Q}_{tr}^{in}$  is the translational energy transported into the wall,  $\bar{Q}_{tr}^{out}$  is the corresponding outgoing energy flux and  $\bar{Q}_{tr}^w$  is the translational energy that would be carried by an emerging stream with the wall temperature. The full boundary condition may now be written

$$\begin{aligned} h_i^+ &= h_{0i} + Ah_i^- \\ h_{0i} &= \tau [\alpha_{tr}(c^2 - 2) + \alpha_{int}(\varepsilon_i - c_v^i/k)] \\ Ah_i^- &= \frac{2}{\pi} \sum_j \frac{e^{-\varepsilon_j}}{Q_0} \int_{\mathbf{c}' \cdot \mathbf{n} < 0} d\mathbf{c}' e^{-c'^2} |\mathbf{c}' \cdot \mathbf{n}| \left\{ 1 + \frac{(1 - \alpha_{tr})}{2} \right. \\ &\quad \times (c^2 - 2)(c'^2 - 2) + (1 - \alpha_{int}) \frac{k}{c_v^j} \left( \varepsilon_i - \frac{c_v^i}{k} \right) \\ &\quad \left. \times \left( \varepsilon_j - \frac{c_v^j}{k} \right) \right\} h_j^-(\mathbf{c}'). \end{aligned} \quad (28)$$

In the limit  $\alpha_{tr} = \alpha_{int} = 1$  this gives the correct result for diffuse emission. The free molecular distribution may be obtained by solving a simple integral equation in this planar geometry as

$$h_i^{FM} = \tau \left[ \frac{\alpha_{tr}}{2 - \alpha_{tr}} (c^2 - 2) + \frac{\alpha_{int}}{2 - \alpha_{int}} \left( \varepsilon_i - \frac{c_v^i}{k} \right) \right] \operatorname{sgn} c_x \quad (29)$$

which is identical to that obtained with Maxwell's assumption. Furthermore the nearly free molecular distribution may be obtained by Knudsen iteration [1] on equation (24) with the free molecular result as the zeroth iterate and is given by

$$\begin{aligned} h_i &= c_x^{-1} \left( x + \frac{\delta}{2} \operatorname{sgn} c_x \right) Lh^{FM} + h^{FM} - \frac{\sqrt{\pi}}{2} \\ &\quad (c^2 - 2, \operatorname{sgn} c \times Lh^{FM}) \left( \frac{1 - \alpha_{tr}}{2 - \alpha_{tr}} \right) (c^2 - 2) \operatorname{sgn} c_x \\ &\quad - \frac{\sqrt{\pi k}}{c_v^i} (\varepsilon_i - c_v^i/k, \operatorname{sgn} c_x Lh^{FM}) \left( \frac{1 - \alpha_{int}}{2 - \alpha_{int}} \right) \\ &\quad \times \left( \varepsilon_i - \frac{c_v^i}{k} \right) \operatorname{sgn} c_x. \end{aligned} \quad (30)$$

Now with the total heat transfer defined as

$$\bar{Q}_{T_x} = \sum_i \int f_i \left( \frac{m\xi^2}{2} + E_i \right) \xi_x d\xi \quad (31)$$

we have, in terms of the inner product (15),

$$\bar{Q}_{T_x} = p_0(2\mathcal{R}T_0)^{\frac{1}{2}} \left[ c_x \left( c^2 - \frac{5}{2} + \varepsilon_i - \frac{c_v^i}{k} \right), h \right] \quad (32)$$

where  $p_0$  is the pressure at  $x = 0$ . Thus the heat transfer to the wall in this limit is

$$\bar{Q}_{T_x} = \bar{Q}_{T_x}^{\text{FM}} \left( 1 + \frac{\pi^{\frac{1}{2}}}{4} b^{-1} I \delta \right) \quad \delta \ll 1 \quad (33)$$

$$\bar{Q}_{T_x}^{\text{FM}} = p_0(2\mathcal{R}T_0)^{\frac{1}{2}} \frac{2\tau}{\pi^{\frac{1}{2}}} b \quad (34)$$

$$b = \frac{\alpha_{\text{tr}}}{2 - \alpha_{\text{tr}}} + \frac{c_v^i}{2k} \frac{\alpha_{\text{int}}}{2 - \alpha_{\text{int}}} \quad (35)$$

$$I = \tau^{-2} (h^{\text{FM}}, Lh^{\text{FM}}). \quad (36)$$

In the continuum limit the solution to (24) is independent of the boundary conditions and is given by the Chapman-Enskog theory as

$$h_i^{\text{asy}} = - \left( \frac{2\tau x}{\delta} \right) \left( c^2 - \frac{5}{2} + \varepsilon_i - \frac{c_v^i}{k} \right) - a_i(c) c_x \frac{2\tau}{\delta} \quad (37)$$

$$L[a_i(c) c_x] = c_x \left( c^2 - \frac{5}{2} + \varepsilon_i - \frac{c_v^i}{k} \right) \quad (38)$$

with the auxiliary condition

$$(a_i(c) c_x, c_x) = 0 \quad (39)$$

and is related to the total thermal conductivity by the relation

$$\lambda_T = - N_0 k (2\mathcal{R}T_0)^{\frac{1}{2}} \left[ a_i(c) c_x, c_x \left( c^2 - \frac{5}{2} + \varepsilon_i - \frac{c_v^i}{k} \right) \right]. \quad (40)$$

Now a trial function which contains a linear combination of both the free molecular and continuum solutions will surely give results for the heat transfer which are correct in both limits

and experience has shown that this is also true for the full transition regime as well. Thus we choose

$$\tilde{h}_i = \beta_1 x \left( c^2 - \frac{5}{2} + \varepsilon_i - \frac{c_v^i}{k} \right) + \beta_2 a_i(c) + \beta_3 \left[ \frac{\alpha_{\text{tr}}}{2 - \alpha_{\text{tr}}} (c^2 - 2) + \frac{\alpha_{\text{int}}}{2 - \alpha_{\text{int}}} \left( \varepsilon_i - \frac{c_v^i}{k} \right) \right] \text{sgn } c_x \quad (41)$$

and use the stationary condition  $\delta J = 0$  to obtain a  $3 \times 3$  system of linear equations for the coefficients. The inclusion of the accommodation coefficients in the trial function enables us to retain the correct free molecular solution without introducing separate variational constants for the internal and translational energies.

Using equation (41) in (22) leads to the system

$$\begin{aligned} & -\beta_1 \left( \alpha_{\text{tr}} + \frac{c_v^i}{2k} \alpha_{\text{int}} \right) \delta \\ & + \beta_2 \left[ \frac{4}{3} J_1 (2 - \alpha_{\text{tr}}) + \frac{4}{3} J_1^* (2 - \alpha_{\text{int}}) \right] \\ & + \beta_3 2 \left( \alpha_{\text{tr}} + \alpha_{\text{int}} \frac{c_v^i}{2k} \right) = 2\tau \left( \alpha_{\text{tr}} + \frac{c_v^i}{2k} \alpha_{\text{int}} \right) \end{aligned} \quad (42.a)$$

$$\begin{aligned} & \beta_1 \delta [J_1 (2 - \alpha_{\text{tr}}) + J_1^* (2 - \alpha_{\text{int}})] \\ & + \beta_2 \left\{ \frac{3}{2} J_2 + \frac{4}{3} \left[ (1 - \alpha_{\text{tr}}) J_1^2 \right. \right. \\ & \left. \left. + (1 - \alpha_{\text{int}}) J_1^{*2} \frac{2k}{c_v^i} \right] - 2\delta (J_1 + J_1^*) \right\} \\ & + \beta_3 [2(\alpha_{\text{tr}} J_1 + \alpha_{\text{int}} J_1^*) - 3\delta b] \\ & = 2\tau (\alpha_{\text{tr}} J_1 + \alpha_{\text{int}} J_1^*) \end{aligned} \quad (42.b)$$

$$\begin{aligned} & \beta_1 \delta \left( \alpha_{\text{tr}} + \frac{c_v^i}{2k} \alpha_{\text{int}} \right) \\ & + \beta_2 \left[ \frac{4}{3} (J_1 \alpha_{\text{tr}} + J_1^* \alpha_{\text{int}}) - 2\delta b \right] \\ & + \beta_3 \left[ 2 \left( \frac{\alpha_{\text{tr}}^2}{2 - \alpha_{\text{tr}}} + \frac{\alpha_{\text{int}}^2}{2 - \alpha_{\text{int}}} \frac{c_v^i}{2k} \right) - \pi^{\frac{1}{2}} \delta I \right] \\ & = 2\tau \left[ \frac{\alpha_{\text{tr}}^2}{2 - \alpha_{\text{tr}}} + \frac{\alpha_{\text{int}}^2}{2 - \alpha_{\text{int}}} \frac{c_v^i}{2k} \right] \end{aligned} \quad (42.c)$$

where we have made the further definitions

$$J_1 = \sum_i \frac{e^{-\epsilon_i}}{Q_0} \int_0^\infty e^{-c^2} c^6 a_i(c) dc \quad (43.a)$$

$$J_1^* = \sum_i \frac{e^{-\epsilon_i}}{Q_0} \int_0^\infty e^{-c^2} c^4 \epsilon_i a_i(c) dc \quad (43.b)$$

$$J_2 = \sum_i \frac{e^{-\epsilon_i}}{Q_0} \int_0^\infty e^{-c^2} c^5 [a_i(c)]^2 dc. \quad (43.c)$$

Using (32) we obtain the heat transfer, normalized to free molecular conditions, in terms of the variational constants directly from the trial function as

$$Q \equiv \frac{\bar{Q}_{Tx}}{\bar{Q}_{Tx}^{FM}} = \frac{2}{3}(\tau b)^{-1} (J_1 + J_1^*) \beta_2 + \tau^{-1} \beta_3 \quad (44)$$

and, after some tedious algebra to obtain the coefficients  $\beta_2$  and  $\beta_3$ , this becomes

$$Q = \frac{N + \delta}{N + M\delta + P\delta^2} \quad (45)$$

where

$$N = \frac{4(J_1 + J_1^*)}{3 - \sqrt{\pi} b^{-2} I (J_1 + J_1^*)}$$

$$\left[ \frac{9}{16(J_1 + J_1^*)^2} - b^{-1} + \frac{G}{2} \right] \quad (46.a)$$

$$M = \frac{3b^2 - \sqrt{\pi} I b (J_1 + J_1^*) \left[ \frac{9}{16(J_1 + J_1^*)^2} + \frac{G}{2} \right]}{3b^2 - \sqrt{\pi} I (J_1 + J_1^*)} \quad (46.b)$$

$$P = -\frac{3b}{4(J_1 + J_1^*)} \quad (46.c)$$

$$G = (J_1 + J_1^*)^{-2} \left[ J_1^2 (1 - \alpha_{tr}) + \frac{2k}{c_v^i} J_1^{*2} (1 - \alpha_{int}) + \left( \alpha_{tr} + \frac{c_v^i}{2k} \alpha_{int} \right)^{-1} [J_1(2 - \alpha_{tr}) + J_1^*(2 - \alpha_{int})]^2 \right]. \quad (46.d)$$

The normalized heat flux given by (45) reduces to the correct values in the limits of large and small inverse Knudsen number. Furthermore the correct initial slope to the heat transfer (or the nearly free molecular correction) is obtained. Thus defining

$$s = \lim_{\delta \rightarrow 0} \frac{d}{d\delta} Q \quad (47)$$

leads to

$$s = \frac{\sqrt{\pi}}{4} b^{-1} I \quad (48)$$

in agreement with the result of equation (30). In the limit of vanishing internal specific heat ( $c_v^i/k \rightarrow 0$ ), equation (45) reduces to the result previously given for the monatomic gas.

### THE TEMPERATURE JUMP

In many practical applications, it is possible to extend the range of validity of the continuum equations by relaxing the "no slip" condition at a solid boundary. In this case it is necessary to have a kinetic treatment of the appropriate slip coefficients. Calculation of these quantities for a monatomic gas is reasonably complete, but the situation for the polyatomic has been less completely treated. It has been shown in a recent treatment, however, that through a redefinition of certain inner products and the collisional invariants, the results previously developed for monatomic gas through use of variational principles may be used directly for polyatomic gases and gas mixtures [25]. Although in shear flow problems it appears the effect of the internal degrees of freedom is slight [7], the transport of energy between the translational and internal modes and the transport of the internal energy itself can have a significant effect in problems in which a temperature gradient exists with a component normal to the solid boundary.

The temperature jump coefficient  $\mathcal{E}$  is usually defined implicitly through the relation

$$T^{asy} \left( -\frac{\delta}{2} \right) - T_w = \mathcal{E} l \frac{dT^{asy}}{d\bar{x}} \quad (49)$$



where  $l$  is the mean free path. With this definition the coefficient of  $l/\bar{\delta}$  in an expansion of the ratio of  $Q$  to its continuum value in powers of  $l/\bar{\delta}$  is simply  $2\mathcal{E}$ . Thus  $\mathcal{E}$  is obtained from equation (45) as

$$\mathcal{E} = \frac{1}{2l} \frac{4}{3} (J_1 + J_1^*) \left\{ \frac{9}{16} \frac{J_2}{(J_1 + J_1^*)^2} + \frac{G}{2} \right\} \quad (50)$$

where the mean free path has been left arbitrary and the terms  $J_1$ ,  $J_1^*$ ,  $J_2$  and  $G$  have been defined in equations (43) and (46). From equation (40) it is noted that  $J_1$  and  $J_1^*$  may be expressed in terms of the translational and internal thermal conductivities as

$$J_1 = -\frac{3}{4} \frac{\lambda_{tr}}{N_0 k} \left( \frac{\pi}{2\mathcal{R}T_0} \right)^{\frac{1}{2}}$$

$$J_1^* = -\frac{3}{4} \frac{\lambda_{int}}{N_0 k} \left( \frac{\pi}{2\mathcal{R}T_0} \right)^{\frac{1}{2}}. \quad (51)$$

Thus introducing the Eucken factors  $F_{tr}$ ,  $F_{int}$  we have

$$G = F_T^{-2} \left\{ F_{tr}^2 (1 - \alpha_{tr}) + F_{int}^2 \frac{2k}{c_v^i} (1 - \alpha_{int}) + \left( \alpha_{tr} + \frac{c_v^i}{2k} \alpha_{int} \right)^{-1} [F_{tr} (2 - \alpha_{tr}) + F_{int} (2 - \alpha_{int})]^2 \right\} \quad (52)$$

$$F_{tr} = \frac{m\lambda_{tr}}{\mu c_v}, \quad F_{int} = \frac{m\lambda_{int}}{\mu c_v}; \quad F_T = F_{tr} + F_{int}. \quad (53)$$

In first Chapman-Enskog approximation,  $a_i(c)$  is given by

$$a_i(c) = a_1(c^2 - 5/2) + a_2(\varepsilon_i - c_v^i/k) \quad (54)$$

where

$$a_1 = -\frac{4}{5} \frac{\lambda_{tr}}{N_0 k} \frac{1}{(2\mathcal{R}T_0)^{\frac{1}{2}}}$$

$$a_2 = -\frac{2\lambda_{int}}{c_v^i N_0 (2\mathcal{R}T_0)^{\frac{1}{2}}} \quad (55)$$

so that the integral  $J_2$  may be evaluated as

$$J_2 = \left[ \frac{52}{25} \lambda_{tr}^2 + 4\lambda_{int}^2 \frac{k}{c_v^i} \right] (N_0 k)^{-2} (2\mathcal{R}T_0)^{-1}. \quad (56)$$

Now choosing the mean free path

$$l = \frac{\mu}{\rho_0} \left( \frac{\pi}{2\mathcal{R}T_0} \right)^{\frac{1}{2}} \quad (57)$$

the temperature slip may be written in terms of the Eucken numbers and the internal heat capacity as

$$\mathcal{E} = \frac{1}{2} \frac{1}{F_T(\gamma - 1)} \left\{ \frac{52}{25\pi} F_{tr}^2 + \frac{4k}{c_v^i} F_{int}^2 + \frac{F_T^2}{2} G \right\} \quad (58)$$

where  $\gamma$  is the ratio of specific heats. Equation (58), in conjunction with experimental determinations of the total Eucken number and the translational Eucken number (e.g. from thermal transpiration data [26]), could serve as an analytical tool in more accurate determinations of the thermal accommodation coefficients.

#### USE OF A MODEL EQUATION

Although the results given in equations (45) and (46) are completely general, the appearance of the half range bracket integral  $I$  of equation (36) makes it necessary to use a modelled collision operator to perform calculations due to the complexity of the collision cross sections. The hierarchy of models of Hanson and Morse [12] is capable of describing collisions between molecules to arbitrary accuracy with the assumption of constant collision frequency. It is well known that constant collision frequency models for monatomic gases in lowest approximation fail to give the correct Prandtl number of the gas, but that an appropriate definition of the mean free path minimizes this discrepancy [4, 5]. The situation for a polyatomic gas is naturally somewhat more complex and it is necessary to truncate the expansion of the collision operator at the next highest order to describe correctly the transport properties, at least in the sense of the first Chapman-Enskog approximation. This

has been discussed in detail elsewhere [12, 27]. At this level the gas may be described in terms of four dimensionless groups. For the heat transfer problem these are chosen to be (1)  $c_v^i/k$  the dimensionless internal specific heat (2)  $z_c$  the collisional relaxation number (to be defined below) (3) the total Eucken number and (4) the inverse Knudsen number based on the plate separation. Equation (24) can now be rewritten as

$$c_x \frac{\partial h}{\partial x} = \hat{L}h \tag{59}$$

where  $\hat{L}$  is the modelled collision operator

$$\begin{aligned} \hat{L}(h_i) = & (1, h_i) + \frac{2}{3}(c^2 - \frac{5}{2}) \\ & \left[ \left( 1 - \frac{2c_v^i}{3k} \frac{1}{z_c} \right) (c^2 - \frac{5}{2}, h_i) + \frac{1}{z_c} \left( \varepsilon_i - \frac{c_v^i}{k}, h_i \right) \right] \\ & \frac{k}{c_v^i} \left( \varepsilon_i - \frac{c_v^i}{k} \right) \left[ \frac{2c_v^i}{3k} \frac{1}{z_c} (c^2 - \frac{5}{2}, h_i) \right. \\ & \left. + \left( 1 - \frac{1}{z_c} \right) \left( \varepsilon_i - \frac{c_v^i}{k}, h_i \right) \right] \\ & + c_x (c^2 - \frac{5}{2}) \left\{ \frac{4}{9} \left( 1 - \frac{c_v^i}{k} \frac{1}{z_c} \right) [c_x (c^2 - \frac{5}{2}), h_i] \right. \\ & \left. + \frac{2}{3} \frac{1}{z_c} \left[ c_x \left( \varepsilon_i - \frac{c_v^i}{k} \right), h_i \right] \right\} \\ & + c_x \left( \varepsilon_i - \frac{c_v^i}{k} \right) \left\{ \frac{2}{3} \frac{1}{z_c} [c_x (c^2 - \frac{5}{2}), h_i] \right. \\ & \left. + (1 - K) \frac{2k}{c_v^i} \left[ c_x \left( \varepsilon_i - \frac{c_v^i}{k} \right), h_i \right] \right\} \tag{60} \end{aligned}$$

and, with the experimental relaxation time  $\tau_R$ , the collision relaxation number has been defined as

$$z_c = \tau_R / \tau_c = \frac{3}{2} p_0 \tau_R / \mu \tag{61}$$

where  $\tau_c$  is chosen to be  $\frac{2}{3} \mu / p_0$  in accord with the total collision frequency as given by the model

equation at this level. Further the quantity  $K$  is given by

$$K = \frac{\frac{10}{9} \frac{c_v^i}{k} \frac{1}{z_c} + \frac{2}{3} \frac{c_v^i}{k} \left( \frac{4}{9} + \frac{5}{9} \frac{c_v^i}{k} \frac{1}{z_c} \right) + \frac{5}{18} \frac{c_v^i}{k} \frac{1}{z_c^2} \frac{c_v}{k} F_T}{\left( \frac{4}{9} + \frac{5}{9} \frac{c_v^i}{k} \frac{1}{z_c} \right) \frac{c_v}{k} F_T - \frac{5}{3}} \tag{62}$$

and the mean free path  $l$  has been chosen in terms of the gas viscosity as

$$l = \frac{4}{3} \frac{\mu}{\rho_0} \frac{1}{(2 \mathcal{A} T_0)^{\frac{1}{2}}} \tag{63}$$

The Chapman-Enskog solution is correctly given, in first approximation, in terms of the model parameters as

$$a_i(c) = a_1(c^2 - \frac{5}{2}) + a_2(\varepsilon_i - c_v^i/k) \tag{64}$$

where

$$a_1 = - \frac{K + \frac{1}{3} \frac{c_v^i}{k} \frac{1}{z_c}}{\left( \frac{4}{9} + \frac{5}{9} \frac{c_v^i}{k} \frac{1}{z_c} \right) K - \frac{8}{45} \frac{c_v^i}{k} \frac{1}{z_c^2}} \tag{65}$$

$$a_2 = - \frac{\left( \frac{4}{9} + \frac{5}{9} \frac{c_v^i}{k} \frac{1}{z_c} \right) - \frac{8}{15} \frac{1}{z_c}}{\left( \frac{4}{9} + \frac{5}{9} \frac{c_v^i}{k} \frac{1}{z_c} \right) K - \frac{8}{45} \frac{c_v^i}{k} \frac{1}{z_c^2}} \tag{66}$$

and are related to the translational and internal thermal conductivities. Now the integrals appearing in the heat transfer may be explicitly computed:

$$J_1 = \frac{15}{16} \pi^{\frac{1}{2}} a_1, \quad J_1^* = \frac{3\pi^{\frac{1}{2}}}{8} \frac{c_v^i}{k} a_2 \tag{67}$$

$$J_2 = \frac{13}{4} a_1^2 + \frac{c_v^i}{k} a_2^2 \tag{68}$$

$$I = \left( \frac{\alpha_t}{2 - \alpha_t} \right)^2 \left[ \frac{16}{9\pi} \left( 1 - \frac{c_v^i}{k} \frac{1}{z_c} \right) - \frac{7}{4} \right]$$

$$+ \frac{8}{3\pi} \frac{c_v^i}{k} \frac{1}{z_c} \left( \frac{\alpha_t}{2 - \alpha_t} \right) \left( \frac{\alpha_{int}}{2 - \alpha_{int}} \right)$$

$$+ \frac{2c_v^i}{\pi k} (1 - K) \left( \frac{\alpha_{\text{int}}}{2 - \alpha_{\text{int}}} \right)^2. \quad (69)$$

With these expressions used in equations (46) in conjunction with equation (45), the heat transfer may be evaluated for arbitrary inverse Knudsen number as a function of the collision relaxation number, the internal specific heat and the total Eucken number of the gas.

### CONCLUSIONS

A variational principle has been used on the full linearized Wang Chang-Uhlenbeck equation in order to describe the heat conducted by a polyatomic gas between two parallel plates. The result is a closed form expression rational in the inverse Knudsen number which correctly gives the free molecular, near free molecular, and continuum heat transfer. In addition a reasonable result has been derived for the temperature jump coefficient which agrees with the monatomic limits and with an independent calculation using the integral form of the equation.

The heat transfer found by the variational method has been expressed in terms of the Chapman-Enskog transport coefficients, in first approximation, by using a modelled collision operator. It is hoped that this expression, in conjunction with experimental values of the gas properties, could be useful in studies of surface accommodation.

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#### TRANSFERT THERMIQUE ET SAUT DE TEMPÉRATURE DANS UN GAZ POLYATOMIQUE

**Résumé**—Afin d'évaluer la chaleur conduite au travers d'un gaz polyatomique entre des plaques parallèles, on utilise un principe variationnel basé sur la forme intrégré-différentielle de l'équation linéarisée de Wang-Chang Uhlenbeck avec des conditions aux limites générales. On donne une expression de forme analytique précise du transfert thermique valable pour tous les degrés de raréfaction rationnelle en fonction de l'inverse du nombre de Knudsen avec pour paramètres les coefficients d'accommodation thermique, la chaleur spécifique des modes internes, les moments de la solution de Chapman Enskog et les intégrales crochets de la solution moléculaire libre. Le coefficient du saut de température est obtenu à partir du développement de haute densité du flux thermique et dépend des coefficients d'accommodation thermique, de la chaleur spécifique interne et des moments de la solution de Chapman Enskog. Dans la limite d'évanouissement de la chaleur spécifique interne, à la fois le transfert thermique et le saut de température se ramènent aux résultats donnés antérieurement pour le gaz monoatomique.

#### WÄRMEÜBERTRAGUNG UND TEMPERATURSPRUNG IN EINEM MEHRATOMIGEN GAS

**Zusammenfassung**—Ein Variationsprinzip, beruhend auf der Integro-Differential-Form der linearisierten Wang-Chang-Uhlenbeck-Gleichung, mit allgemeinen Randbedingungen, wurde zum Berechnen der Wärmeleitung durch ein mehratomiges Gas zwischen parallelen Platten benutzt. Das Ergebnis ist ein genauer, geschlossener Ausdruck für die Wärmeübertragung, gültig für alle Verdünnungsgrade, rational in der inversen Knudsenzahl und parametrisiert durch die thermischen Akkommodationskoeffizienten, die Wärmekapazität der inneren Zustände, die Gesamtmomente aus der Chapman-Enskog-Lösung und Halb-Bereichs-Stützintegrale aus der Lösung für frei bewegliche Moleküle. Der Temperatursprungkoeffizient ist gewonnen aus der hohen Dichtezunahme infolge des Wärmestromes und ist abhängig von den thermischen Akkommodationskoeffizienten, der inneren Wärmekapazität und den Momenten aus der Chapman-Enskog-Lösung.

Im Grenzfall des Verschwindens der inneren spezifischen Wärme reduzieren sich die Ergebnisse für die Wärmeübertragung und den Temperatursprung auf die früher bestimmten Ergebnisse für das einatomige Gas.

#### ПЕРЕНОС ТЕПЛА И ТЕМПЕРАТУРНЫЙ СКАЧОК В МНОГОАТОМНОМ ГАЗЕ

**Аннотация**—Для оценки количества тепла, переданного теплопроводностью через разреженный газ, заключенный между параллельными пластинами, используется вариационный принцип решения линейризованного интегро-дифференциального уравнения Вань-Чань-Уленбека с общими граничными условиями. Получено выражение для потока тепла, справедливое для всех степеней разрежения, т.е. для любых  $(Kn)^{-1}$ , и содержащее в качестве параметров коэффициенты термической аккомодации теплоемкость за счёт внутренних степеней свободы, полный набор моментов функции распределения, согласно процедуре решения Чепмена-Энскога, и ряд интегралов столкновений. Выражение для температурного скачка получено разложением выражения для теплового потока в ряд по плотности и зависит от коэффициентов термической аккомодации, теплоемкости за счёт внутренних степеней свободы и моментов решения Чепмена-Энскога. В пределе при стремлении теплоемкости за счёт внутренних степеней свободы к нулю, выражения как для теплового потока, так и для температурного скачка, совпадают с аналогичными выражениями в случае одноатомного газа.