



The role of the dynamic pressure in stationary heat conduction of a rarefied polyatomic gas



Takashi Arima^a, Elvira Barbera^b, Francesca Brini^{c,*}, Masaru Sugiyama^d

^a Department of Mechanical Engineering, Faculty of Engineering, Kanagawa University, Yokohama 221-8686, Japan

^b Department of Mathematics and Computer Science, University of Messina, V.le F. D'Alcontres 31, 98166 Messina, Italy

^c Department of Mathematics, University of Bologna, via Saragozza 8, 40123 Bologna, Italy

^d Graduate School of Engineering, Nagoya Institute of Technology, Nagoya 466-8555, Japan

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ABSTRACT

The effect of the dynamic pressure (non-equilibrium pressure) on stationary heat conduction in a rarefied polyatomic gas at rest is elucidated by the theory of extended thermodynamics. It is shown that this effect is observable in a non-polytropic gas. Numerical studies are presented for a para-hydrogen gas as a typical example.

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1. Introduction

Heat conduction is one of the basic non-equilibrium phenomena already studied by many researchers, although several fundamental questions remain still open. In the present Letter, we study the stationary heat transfer in a *rarefied polyatomic* gas at rest, confined in a bounded domain in planar or radial geometry. To our knowledge, this is the first analysis of heat conduction in which the effect of the dynamic pressure is investigated. As is well known, the dynamic pressure vanishes identically in a rarefied monatomic gas, while it is intrinsically related to the internal degrees of freedom of the polyatomic molecules. Therefore, what we will analyze here is a *polyatomic effect*.

In the literature on heat conduction in such gases, the theoretical studies have been carried out mainly based on the kinetic theory, for example, see Ref. [1]. However, for the heat conduction problem in particular, the role of the dynamic pressure has been always overlooked, although the dynamic pressure has been actively discussed in literature starting from Leontovich and Mandelshtam [2,3] (see also Refs. [4,5], Section 78 of Ref. [6] and Chap-

ter 12 of Ref. [7]) and has been studied in various phenomena, for example, dispersion of sound waves [7], reacting gas flows [8,9]. In addition, the kinetic theory encounters serious difficulty in the modeling of the collision term between polyatomic molecules of gases in which the internal modes play an important role.

The experimental studies for polyatomic gases have been presented only in the case of a nitrogen (N_2) gas in [10], where a highly rarefied gas is confined between two parallel plates kept at different temperatures. In that paper, the mass density is measured inside the device through a luminescence technique, while the total heat flux is presented as a function of the inverse of the Knudsen number (the ratio between the mean free path of a molecule and the characteristic length of the domain).

In order to achieve our aim, we adopt the extended thermodynamics (ET) theory [11] because, as shown later, the classical Navier–Stokes Fourier (NSF) theory [7,6] is insufficient for the description of the phenomena under consideration. The ET theory has been constructed in a phenomenological way in which the spatio-temporally local constitutive equations are severely restricted by imposing the universal physical principles and therefore this theory is free from the difficulty of the kinetic theory. We recall that, also for monatomic gases, ET and NSF carry mutually different results in the heat transfer problem both for single gases (see [12–14] and the references therein) and for gas mixtures [15–17]. Here, we will use an ET theory with 14 independent fields (ET14)

* Corresponding author.

E-mail addresses: arima@kanagawa-u.ac.jp (T. Arima), ebarbera@unime.it (E. Barbera), francesca.brini@unibo.it (F. Brini), sugiyama@nitech.ac.jp (M. Sugiyama).

[18–20]. These 14 fields have well-established macroscopic physical meanings and also appear in the NSF theory, while the meanings of the higher moments which are discussed in the theory of moment equations [21,22] are usually difficult to be grasped.

ET14 has been already applied successfully to various subjects: heat conduction in a van der Waals fluid [23], sound waves [24,25], light scattering [26] and shock waves [27–29]. From the kinetic theory, it was also proven [30] that ET14 is perfectly consistent with molecular ET with the method of closure by the maximum entropy principle [31–33].

In this Letter, we will study heat conduction in *non-polytropic* rarefied gases and present as a numerical example the *para-hydrogen* (p-H₂) gas case.

2. ET14 theory

The ET14 theory is a phenomenological continuum theory for both dense and rarefied polyatomic gases [18–20]. The theory adopts the binary hierarchy of the balance equations with the 14 independent field variables: the mass density ρ , the velocity v_i , the temperature T , the shear stress $S_{(ij)}$ (symmetric traceless part of the viscous stress S_{ij}), the dynamic pressure Π ($= -S_{ii}/3$), and the heat flux q_i , where $i, j = 1, 2, 3$. Here and hereafter summation on repeated indices is assumed. The stress tensor is given by $t_{ij} = -p\delta_{ij} + S_{ij}$ if p denotes the equilibrium pressure and δ is the Kronecker symbol. All these field variables take part also in the NSF theory.

Usually in ET the constitutive equations are determined through the validity of general principles: the objectivity principle (that is, the material frame indifference principle and the Galilean invariance for the balance equations), the entropy principle (the second law of thermodynamics), and the causality principle. For this problem, as shown in [11], the constitutive equations are explicitly expressed by the equilibrium thermal and caloric equations of state. In the present study, we adopt the equations of state for a *classical* (i.e., non-degenerate) ideal gas expressed by

$$p = \frac{k_B}{m} \rho T, \quad \varepsilon = \varepsilon(T), \quad (1)$$

where ε , k_B and m are, respectively, the specific internal energy, the Boltzmann constant and the mass of a molecule. Note that the gas under consideration could be, in general, non-polytropic, that is, its specific heat at constant volume $c_v (= d\varepsilon/dT)$ could be a non-constant function of the temperature.

The closed system of field equations in the Cartesian coordinate system is given by

$$\begin{aligned} \dot{\rho} + \rho \frac{\partial v_k}{\partial x_k} &= 0, \\ \rho \dot{v}_i + \frac{\partial p}{\partial x_i} + \frac{\partial \Pi}{\partial x_i} - \frac{\partial S_{(ij)}}{\partial x_j} &= 0, \\ \rho \frac{k_B}{m} \hat{c}_v \dot{T} + (p + \Pi) \frac{\partial v_k}{\partial x_k} - \frac{\partial v_i}{\partial x_k} S_{(ik)} + \frac{\partial q_k}{\partial x_k} &= 0, \\ \hat{S}_{(ij)} - 2(p + \Pi) \frac{\partial v_{(i}}{\partial x_{j)}} + S_{(ij)} \frac{\partial v_k}{\partial x_k} + 2 \frac{\partial v_{(i}}{\partial x_k} S_{(j)k)} & \\ + \frac{2}{(1 + \hat{c}_v)^2} \frac{d\hat{c}_v}{dT} \frac{\partial T}{\partial x_k} q_{(i} \delta_{j)k} - \frac{2}{1 + \hat{c}_v} \frac{\partial q_{(i}}{\partial x_{j)}} &= -\frac{1}{\tau_S} S_{(ij)}, \\ \dot{\Pi} + \left(\left(\frac{2}{3} - \frac{1}{\hat{c}_v} \right) p + \left(\frac{5}{3} - \frac{1}{\hat{c}_v} \right) \Pi \right) \frac{\partial v_k}{\partial x_k} + \left(\frac{1}{\hat{c}_v} - \frac{2}{3} \right) \frac{\partial v_{(i}}{\partial x_{k)}} S_{(ik)} & \\ - \frac{5}{3} \frac{1}{(1 + \hat{c}_v)^2} \frac{d\hat{c}_v}{dT} q_k \frac{\partial T}{\partial x_k} + \frac{2\hat{c}_v - 3}{3\hat{c}_v(1 + \hat{c}_v)} \frac{\partial q_k}{\partial x_k} &= -\frac{1}{\tau_\Pi} \Pi, \end{aligned}$$

$$\begin{aligned} \dot{q}_i + \frac{2 + \hat{c}_v}{1 + \hat{c}_v} q_i \frac{\partial v_k}{\partial x_k} + \frac{1}{1 + \hat{c}_v} q_k \frac{\partial v_k}{\partial x_i} + \frac{2 + \hat{c}_v}{1 + \hat{c}_v} q_k \frac{\partial v_i}{\partial x_k} & \\ - \frac{k_B}{m} T \frac{\partial p}{\partial x_k} + \frac{k_B}{m} ((1 + \hat{c}_v)p \delta_{ki} + (2 + \hat{c}_v)(\Pi \delta_{ki} - S_{(ki)})) \frac{\partial T}{\partial x_k} & \\ + \frac{1}{\rho} ((p - \Pi) \delta_{ki} + S_{(ki)}) \frac{\partial}{\partial x_i} ((p + \Pi) \delta_{kl} - S_{(kl)}) & \\ = -\frac{1}{\tau_q} q_i, & \quad (2) \end{aligned}$$

where a dot on a quantity indicates the material time derivative: $(\dot{}) \equiv \partial()/\partial t + v_i \partial()/\partial x_i$; \hat{c}_v is the dimensionless specific heat:

$$\hat{c}_v = \frac{c_v}{k_B/m}; \quad (3)$$

the relaxation times τ_S, τ_Π and τ_q are in general functions of ρ and T .

ET14 contains the NSF theory as a special case in the limit of small relaxation times. By the Maxwellian iteration [11,18,34], τ_S, τ_Π and τ_q evaluated at a reference equilibrium state are related to the shear viscosity μ , the bulk viscosity ν and the heat conductivity κ :

$$\mu = p\tau_S, \quad \nu = \left(\frac{2}{3} - \frac{1}{\hat{c}_v} \right) p\tau_\Pi, \quad \kappa = (1 + \hat{c}_v) \frac{k_B}{m} p\tau_q. \quad (4)$$

For the sake of simplicity, in the present Letter we assume that the relaxation times have constant values, prescribed by the density and the temperature range under consideration.

3. Basis of the present analysis

We confine our study within stationary one-dimensional heat transfer problem in a gas at rest, referring to planar or cylindrical or spherical geometry. All relevant physical quantities will be expressed in terms of the *physical components* [35].

3.1. Basic system of equations

We adopt the following dimensionless quantities:

$$\begin{aligned} \hat{x} &= \frac{x}{L}, \quad \hat{c}'_v = T_0 \frac{d\hat{c}_v}{dT}, \quad \hat{\rho} = \frac{\rho}{\rho_P}, \quad \hat{T} = \frac{T}{T_0}, \quad \hat{p} = \frac{p}{p_P}, \\ \hat{S}_{(ij)} &= \frac{S_{(ij)}}{p_P}, \quad \hat{\Pi} = \frac{\Pi}{p_P}, \quad \hat{q}_1 = \frac{q_1}{p_P \sqrt{k_B T_0/m}}, \\ \hat{\tau}_S &= \frac{\tau_S \sqrt{k_B T_0/m}}{L}, \quad \hat{\tau}_\Pi = \frac{\tau_\Pi \sqrt{k_B T_0/m}}{L}, \\ \hat{\tau}_q &= \frac{\tau_q \sqrt{k_B T_0/m}}{L}, \end{aligned} \quad (5)$$

where x represents the position along the axis normal to the plates in the planar case or the radius in the radial geometries, L is the distance between the two boundaries, ρ_P and T_0 denote some reference values for temperature and pressure, and $p_P = (k_B/m)\rho_P T_0$. It is interesting to note that the dimensionless relaxation time $\hat{\tau}_S$ is proportional to the Knudsen number Kn . Then, for the sake of simplicity, we may assume $Kn = \hat{\tau}_S$.

System (2) becomes:

$$\begin{aligned} \frac{d}{d\hat{x}} (\hat{p} + \hat{\Pi} - \hat{S}_{(11)}) - \frac{j(j+1)}{2\hat{x}} \hat{S}_{(11)} - \frac{j(j-2)}{\hat{x}} \hat{S}_{(22)} &= 0, \\ \frac{d\hat{q}}{d\hat{x}} + \frac{j}{\hat{x}} \hat{q} &= 0, \\ \frac{2}{1 + \hat{c}_v} \frac{d\hat{q}}{d\hat{x}} - \frac{4}{3} \frac{\hat{c}'_v}{(1 + \hat{c}_v)^2} \hat{q} \frac{d\hat{T}}{d\hat{x}} &= \frac{\hat{S}_{(11)}}{\hat{\tau}_S}, \end{aligned}$$

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