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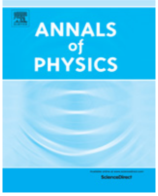

Molecular extended thermodynamics of rarefied polyatomic gases and wave velocities for increasing number of moments

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HIGHLIGHTS

- Molecular extended thermodynamics of rarefied polyatomic gases is studied.
- The relation between two hierarchies of equations for moments is derived.
- The equivalence of maximum entropy principle and entropy principle is proven.
- The characteristic velocities are compared to those of monatomic gases.
- The lower bound of the maximum characteristic velocity is estimated.

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ABSTRACT

Molecular extended thermodynamics of rarefied polyatomic gases is characterized by two hierarchies of equations for moments of a suitable distribution function in which the internal degrees of freedom of a molecule is taken into account. On the basis of physical relevance the truncation orders of the two hierarchies are proven to be not independent on each other, and the closure procedures based on the maximum entropy principle (MEP) and on the entropy principle (EP) are proven to be equivalent.

The characteristic velocities of the emerging hyperbolic system of differential equations are compared to those obtained for monatomic gases and the lower bound estimate for the maximum equilibrium characteristic velocity established for monatomic gases (characterized by only one hierarchy for moments with

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truncation order of moments N) by Boillat and Ruggeri (1997)

$$\frac{\lambda^{E,\,\max}_{(N)}}{c_0} \geqslant \sqrt{\frac{6}{5}\left(N-\frac{1}{2}\right)}, \qquad \left(c_0=\sqrt{\frac{5}{3}\frac{k}{m}T}\right)$$

is proven to hold also for rarefied polyatomic gases independently from the degrees of freedom of a molecule.

1. Introduction

Two complementary approaches, namely the *continuum approach* and the *kinetic approach*, have been used to tackle the challenging task of modeling non-equilibrium phenomena in which steep gradients and rapid changes occur.

The continuum model consists in describing the system by means of macroscopic equations (e.g. fluid-dynamic equations) obtained on the basis of conservation laws and appropriate constitutive equations. As an example, Thermodynamics of Irreversible Processes (TIP), which relies on the assumption of local thermodynamic equilibrium (LTE), has proven to be a useful and sound theory characterized by a systematic and comprehensive theoretical structure [1].

In this framework, the Navier–Stokes–Fourier (NSF) theory [1,2] has gained much popularity mainly due to its practical usefulness in many applications. Nonetheless, TIP and NSF suffer from some limits: since the mathematical structure of these theories is characterized by a system of differential equations of parabolic type, an infinite speed is predicted for the propagation of the signals—an issue which has been addressed as the "paradox of heat conduction" [3]. Moreover, the applicability of the classical macroscopic theory is inherently restricted to processes characterized by *small* Knudsen numbers (i.e. dense gases), and the transport coefficients associated to the dissipation processes are not provided by the theory except for the sign.

On the other hand, the approach based on the kinetic theory, which postulates that the state of the gas can be described by a velocity distribution function whose evolution is governed by the celebrated Boltzmann equation, is applicable to processes characterized by a *large* Knudsen number, and transport coefficients naturally emerge from the theory itself. Nevertheless the range of applicability of the Boltzmann equation is limited to rarefied and monatomic gases.

Extended thermodynamics is a phenomenological theory whose aim is to bridge the gap between these two limit cases.

The first approach to extended thermodynamics (ET), proposed by Müller [4], was based on the modification of the Gibbs relation. This point of view has been adopted by several authors and a survey of these results can be found in the book of Jou, Casas Vásquez and Lebon [5]. This approach was criticized by Ruggeri [6] and later a revision of ET was proposed by Liu and Müller [7] in a classic context, and by Liu, Müller and Ruggeri in a relativistic framework [8]. This new approach was named Rational Extended Thermodynamics (RET) and the main results are the subject of the book of Müller and Ruggeri [9].

The mathematical framework of RET consists of a hierarchy of balance laws having the same structure as the moments of the distribution function of the Boltzmann equation truncated at some arbitrary order of moments N. The theory, under this respect, resembles the kinetic approach, except that the closure is achieved by means of the universal principles of continuum theory: the *entropy principle*, the *objectivity principle* and the *principle of causality and stability*.

The prototype of RET is the so-called "13-*moment theory*" for rarefied mono-atomic gases [7]: following the guidelines of RET, in this case the hierarchy of moments provides the balance laws from which the time evolution of the mass density, velocity, energy, shear stress and heat flux can be obtained. The 13-moment theory turns out to be equivalent to the well-established Grad's moment