AN ADVANCED KINETIC THEORY FOR MORPHING CONTINUUM WITH INNER STRUCTURES

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Advanced kinetic theory with the Boltzmann-Curtiss equation provides a promising tool for polyatomic gas flows, especially for fluid flows containing inner structures, such as turbulence, polyatomic gas flows and others. Although a Hamiltonian-based distribution function was proposed for diatomic gas flow, a general distribution function for the generalized Boltzmann-Curtiss equations and polyatomic gas flow is still out of reach. With assistance from Boltzmann’s entropy principle, a generalized Boltzmann-Curtiss distribution for polyatomic gas flow is introduced. The corresponding governing equations at equilibrium state are derived and compared with Eringen’s morphing (micropolar) continuum theory derived under the framework of rational continuum thermomechanics. Although rational continuum thermomechanics has the advantages of mathematical rigor and simplicity, the presented statistical kinetic theory approach provides a clear physical picture for what the governing equations represent.

Keywords: rational continuum mechanics, kinetic theory, morphing continuum.

1. Introduction

The Navier-Stokes equations have been extensively used to study fluid flow physics for several decades. In the fluid mechanics society, it is usually believed that the Navier-Stokes equations are derived from kinetic theory [1] under the assumption that the system of monatomic gases is nearly in a Boltzmann distribution (equilibrium). A system of monatomic gases in equilibrium defines all the physical quantities in the Boltzmann distribution. For example, the Navier-Stokes equations can be derived from the Boltzmann distribution with a first order approximation applied to the Boltzmann transport equations.

Alternatively, beginning in the early 1960s, Eringen [2,3], Truesdell [4,5] and others [6–8] applied rational continuum thermomechanics, with its mathematical rigor, to investigate continuum theories in solids, fluids, mixtures [9,10] and electrodynamics. The foundation of rational continuum thermomechanics starts with a set of balance...
laws, including continuity, linear momentum, angular momentum, and energy conservation equations. With the assistance of several axioms, such as objectivity (also known as frame-indifference), memory, etc., and the Coleman-Noll procedure [11] based on the Clausius-Duhem inequality (entropy principle), constitutive equations for a fluid can be derived. The combination of balance laws and constitutive equations for fluids from this approach can also lead to the Navier-Stokes equations [3, 4, 6].

Most of the complex fluid flows contain structures across multiple spatial length scales and are usually dominated by the subscale motions. For example, the rotational eddies characterizes the turbulence physics at bulk scale. In addition, most gases are either diatomic or polyatomic. At high altitude or during speed flights, the rotation and vibration of the diatomic/polyatomic molecules causes non-equilibrium flow phenomena extensively. Those flows are known for not being able to be analyzed by the classical continuum mechanics or Navier-Stokes equations. As a result, the continuum theory used to model these flows with subscale or inner structures shall be categorized as morphing continuum.

Although rational continuum thermomechanics provides mathematical rigor to the theoretical formulation, it leaves the physical meanings of material constants in resulting fluid equations unexplained. It is common for practitioners of the rational continuum thermomechanics approach to interpret the material constants through experiments. In contrast, the kinetic theory approach gives physical meaning to the quantities in the fluid equations by the means of the collision and distribution functions. Due to the lack of mathematical rigor in the kinetic theory approach, Truesdell commented that all equations derived from kinetic theory can be considered only as a class of constitutive equations in rational continuum thermomechanics [12]. Although this comment may be true, the physics hidden in all proposed governing equations derived from kinetic theory can be used to interpret the same equations using the rigorous procedure of rational continuum thermomechanics. Such is the purpose of this paper.

Despite the successes of the Navier-Stokes equations derived by both kinetic theory and rational continuum thermomechanics, the derivations have been limited to monatomic gases or rather, volumeless point particles. Inspired by the rigor of rational continuum thermomechanics, Eringen was the first to mathematically formulate the micropolar continuum theory with independent inner structures [13, 14]. This work was later expanded by Chen et. al. for nonlinear constitutive equations for fluids with electromagnetic interactions [7]. Through the multiscale formulation coupling macroscale and subscale motions, this morphing continuum theory successfully reproduces and explains turbulence physics [15–18], polyatomic gases [19] and microfluids [20, 21] which cannot be explained by the classical Navier-Stokes theories. Nevertheless, a disadvantage of the rational continuum thermomechanics approach is that the physical interpretations of the material constants in MCT are still unknown. Consequently, researchers rely on dimension analysis to decipher the underlying physics. Wonnell and Chen presented a systematic derivation on Eringen’s micropolar theory for incompressible turbulence and found a dimensionless parameter differentiating laminar, transition and turbulent flows. One could also rely on advanced kinetic theory to deduce the physical meanings of these MCT material constants. This would be done in a process similar to the one used to de-
rivate the Navier-Stokes equations. This newly introduced advanced kinetic theory would go beyond the classical formulation, which is limited to monatomic gases, and be able to treat polyatomic gases.

The Boltzmann equation was originally developed for a gas consisting of point particles (i.e., a monatomic gas) and was based on physical arguments \[22, 23\]. Curtiss later expanded Boltzmann’s original formulation to diatomic gas molecules \[24\] and polyatomic gas molecules \[23\] to obtain what are known as the Boltzmann-Curtiss equations. Although Eu and Ohr \[25\] proposed a Hamiltonian-based distribution function for diatomic gases using Curtiss’ transport equation proposed in 1981 \[24\], most studies of the Boltzmann-Curtiss equation adopt the classic Boltzmann distribution with approximations \[26, 27\]. This leads to one major question remaining unanswered; namely, what is the distribution that should be used for the generalized Boltzmann-Curtiss equation \[23\]? In this study, a general Boltzmann-Curtiss distribution function (Appendix A) that accounts for the translation and rotation of molecular gases is presented. The corresponding governing equations at equilibrium state are derived and compared with Eringen’s morphing (Micropolar) continuum theory.

Section 2 then introduces an advanced kinetic theory with a general distribution function, which accounts for bulk scale translational velocities and subscale rotational motions, the Boltzmann-Curtiss distribution, and the resulting transport equations. Section 3 shows the pathway to the inviscid version of morphing continuum theory from advanced kinetic theory (see Section 2) and then compares it to the set of equations obtained from rational continuum thermomechanics. Section 4 finally gives a brief discussion about the current study and the next steps.

2. Advanced Kinetic Theory

2.1. Transport Equations

The Boltzmann equation and kinetic theory have been considered as the fundamental equations of hydrodynamics and combine atomic-level physics with statistical averaging. It is well known that the Navier-Stokes equations can be deduced from kinetic theory and the Boltzmann equations using a first order approximation. However, it should be emphasized that the original Boltzmann equation and kinetic theory are based on a monatomic particle assumption. Therefore, more ad hoc approximations have to be made for diatomic or polyatomic molecular gases. Assuming the dynamics of the collisions do not depend on the vibrational energy, Curtiss extended the original formulations for the Boltzmann equation and found the generalized Boltzmann equation (Boltzmann-Curtiss equation) as \[23, 24\]

\[
\bar{f}(x, p, \phi, M, t) = \int f(x, p, \phi, M, E_{\text{vib}}, \tau, t) dE_{\text{vib}} d\tau,
\]

\[
\left(\frac{\partial}{\partial t} + \frac{p}{m} \frac{\partial}{\partial x} + \frac{M}{T} \frac{\partial}{\partial \phi}\right) \bar{f} = \sum_{\beta} Z_{\beta},
\]

(1)
where \( x \) is the position, \( p \) the linear momentum, \( \phi \) the orientation, \( M \) the angular momentum, \( Z \) the collision integral integrated over \( \beta \) molecules that interact with a given molecule, and \( I \) the moment of inertia. It should be noted that Curtiss did not provide a distribution function for the Boltzmann-Curtiss equations. This study presents a distribution that works well with the Boltzmann-Curtiss equations.

### 2.2. Boltzmann-Curtiss Distribution Function

Let \( \chi \) be any conserved kinetic variable associated with a molecule of velocity \( v \) and angular velocity \( \omega \) located at \( x \), such that in any collision at \( x \) one has \( \{p_1, \omega_1, p_2, \omega_2\} \rightarrow \{p'_1, \omega'_1, p'_2, \omega'_2\} \) so that \( \chi_1 + \chi_2 = \chi'_1 + \chi'_2 \) where \( \chi(x, p, \omega) \). The conservation theorem relevant to the Boltzmann-Curtiss equation can be obtained by multiplying Eq. (1) on both sides by \( \chi \) and integrating over \( v' \) and \( \omega' \). The collision term vanishes and the average value, \( \langle A \rangle \), is obtained as

\[
\langle A \rangle \equiv \frac{\int d^3v' d^3\omega' A \bar{f}}{\int d^3v' d^3\omega' \bar{f}} = \frac{1}{n} \int d^3v' d^3\omega' A \bar{f},
\]

where \( n(x, t) \equiv \int d^3v' d^3\omega' \bar{f}(x, p, \omega, t) \).

Assume the inner structure as a rigid sphere and has no distribution inside the molecule, i.e. \( \frac{\partial}{\partial \phi} k = 0 \). In the absence of body force and couple moment, the conservation equation is

\[
\frac{\partial}{\partial t} \langle n \chi \rangle + \frac{\partial}{\partial x_i} \langle n \chi v_i \rangle - n \langle v_i \frac{\partial \chi}{\partial x_i} \rangle - n \langle \chi \frac{\partial v_i}{\partial \phi_i} \rangle = 0,
\]

\[
\Rightarrow \frac{\partial}{\partial t} \langle n \chi \rangle + \frac{\partial}{\partial x_i} \langle n \chi v_i \rangle - n \langle v_i \frac{\partial \chi}{\partial x_i} \rangle = 0
\]

(3)

and the derivation of the Boltzmann-Curtiss distribution can be found in Appendix A. The Boltzmann-Curtiss distribution is

\[
\bar{f}(x, v, \omega) = n \left( \frac{m \sqrt{j}}{2 \pi k \theta} \right)^3 \exp \left[ -\frac{m(v'^2 + j \omega'^2)}{2k\theta} \right].
\]

(4)

The corresponding probability density function has the proper normalization, i.e.,

\[
\int_{-\infty}^{\infty} \left( \frac{m \sqrt{j}}{2 \pi k \theta} \right)^3 \exp \left[ -\frac{m(v'^2 + j \omega'^2)}{2k\theta} \right] d^3v' d^3\omega' = 1.
\]

(5)

Here \( m \) is the mass of the molecule, \( j \) is the microinertia for the inner structure and \( k \) is the Boltzmann constant. One can understand microinertia through the concept of moment of inertia. Microinertia is a measurement of the resistance of the internal structure to changes to its rotation and can be defined as

\[
j \equiv 2\langle r_m r_m \rangle = 2 \int_{\Delta v'} \rho' r_m r_m dv' \int_{\Delta v'} \rho' dv',
\]

(6)
where \( r_m \) is the local coordinate from the centroid of the internal structure and \( \Delta v' \) is the volume of the inner structure.

It should be noted that following the equipartition of energy, \( E_{\text{int}} = \frac{1}{2} N_{\text{DOF}} n k \theta \), the internal energy can be shown to be

\[
E_{\text{int}} = \frac{6}{2} n k \theta = \frac{1}{2} m \left( \langle v'^2 \rangle + j \langle \omega'^2 \rangle \right),
\]

where \( N_{\text{DOF}} \) is the number of the degrees of freedom in a polyatomic molecule and \( n \) is the number of the molecules in the system. The velocity \( v_i \) and the angular velocity \( \omega_i \) can be decomposed as \( v_i = U_i + v_i' \) and \( \omega_i = W_i + \omega_i' \).

2.3. Kinetic Variables

The equations for fluid dynamics involving particles with inner structure can be derived by calculating the moments of the Boltzmann-Curtiss equations for quantities that are conserved in collisions of the molecules. There are four conserved quantities \( \chi \), i.e., the mass \( \chi_1 = m \), the total linear momentum \( \chi_2 = mv^*_i = m(v_i + e_{ijk}\omega_jr_k) \), the angular momentum \( \chi_3 = mj\omega_m \) and the total energy \( \chi_4 = \frac{1}{2} m(v_i v_i + j\omega_i \omega_j) \).

2.3.1. Balance Law of Mass

If \( \chi_1 = m \) is chosen and inserted into Eq. 3, one obtains

\[
\frac{\partial}{\partial t} \langle nm \rangle + \frac{\partial}{\partial x_i} \langle nmv_i \rangle = 0,
\]

With \( nm = \rho \) and \( \langle v_i \rangle = U_i \), the continuity equation is obtained as

\[
\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_i} (\rho U_i) = 0.
\]

2.3.2. Balance Law of Linear Momentum

If \( \chi_2 = mv^*_i = m(v_i + e_{ijk}\omega_jr_k) \), Eq. 3 becomes

\[
\frac{\partial}{\partial t} \langle nmv_j \rangle + \frac{\partial}{\partial x_i} (nme_{jmn}\omega_mr_n) + \frac{\partial}{\partial x_i} \langle nmv_i v_j \rangle
\]

\[
+ \frac{\partial}{\partial x_i} \langle nme_{jmn}\omega_m r_nv_i \rangle = 0,
\]

or

\[
\frac{\partial}{\partial t} \rho U_j + \frac{\partial}{\partial x_i} (\rho U_i U_j) = -\frac{\partial}{\partial x_i} \left( \rho \langle v'_i v'_j \rangle + \rho e_{jmn} r_n \langle v'_i \omega'_m \rangle \right).
\]

Here \( U^*_j = U_j + e_{jmn} W_m r_n \) is the total averaged velocity with the fluctuating velocity integrated over the volume of the molecule being zero, i.e., \( \int e_{jmn} W_m r_n d^3\mathbf{v}' d^3\omega' = 0 \).

The quantity \( t_{ij}^{\text{Boltzmann}} = \rho \langle v'_i v'_j \rangle \) is the stress similar to that in the classical Boltzmann
equation and \( t_{ij}^{\text{Curtiss}} = \rho e_{jmn} \langle v'_m v'_n \rangle \) is the asymmetric part of the stress due to the rotation discussed by Curtiss [23], Eringen [14, 28], Stokes [29] and others [7]. It should be noticed that the integral for the symmetric part of the stress, \( t_{ij}^{\text{Boltzmann}} \), is different from the one in the classical Boltzmann equation due to the distribution function used; however, the derivation still yields the gas pressure and the classical symmetric stress tensor at Boltzmann-Curtiss distribution, namely

\[
t_{ij}^{\text{Boltzmann}} = p \delta_{ij} - t_{ij}^{\text{Boltzmann,viscous}} = \rho \langle v'_i v'_j \rangle
\]

\[
= \frac{\rho}{n} \int m v'_i v'_j \left( \frac{m(j)\pi}{2\pi k\theta} \right)^3 e^{-\frac{(v'^2_i + v'^2_j)}{2nk\theta}} d^3\omega'.
\]

(11)

It is also straightforward to prove that \( \rho \langle v'_i v'_j \rangle = \rho \langle v'_i v'_j \rangle = \rho \langle v'_i v'_j \rangle = nk\theta \) and define the gas pressure as \( p \equiv \frac{1}{3} \rho \langle v'^2 \rangle \) when the system is at the Boltzmann-Curtiss distribution.

### 2.3.3. Balance Law of Angular Momentum

For a rotating body, one of the important quantities is angular momentum. Therefore, the third kinetic variable is \( \chi_3 = mj\omega_m \), where \( j \) is the inertia of the subscale structure.

With the substitution of \( \chi_3 \), Eq. (3) becomes

\[
\frac{\partial}{\partial t} \langle nm j \omega_m \rangle + \frac{\partial}{\partial x_i} \langle nm j \omega_m v_i \rangle = 0
\]

or

\[
\frac{\partial}{\partial t} (\rho j W_m) + \frac{\partial}{\partial x_i} (\rho j W_m U_i) = - \frac{\partial}{\partial x_i} (\rho j \langle \omega'_m v'_i \rangle),
\]

(12)

where the right-hand term, \( m_{im} = \rho j \langle \omega'_m v'_i \rangle \), is the combination of the moment stress due to rotation and the asymmetric part of the Cauchy stress, \( t_{ij}^{\text{Curtiss}} = \rho e_{jmn} \langle v'_m v'_n \rangle \).

### 2.3.4. Balance Law of Energy

In classical kinetic theory, the internal energy density is defined as \( e = \frac{1}{2} \langle v'_m v'_m \rangle \); however, because of the rotating effect of the molecule, the internal energy density should be re-defined as \( e = \frac{1}{2} \langle (v'_m v'_m) + j \langle \omega'_m \omega'_m \rangle \rangle \). Similarly, the total energy is classically defined as \( \frac{1}{2} m \langle v_m v_m \rangle \), but due to the rotation effects of the molecule it should now be defined as \( \frac{1}{2} m \langle v_m v_m + j \omega_m \omega_m \rangle \). This can also be stated as \( \frac{1}{2} m (e + U_m U_m + j W_m W_m) \). After inserting the last kinetic variable, i.e., total energy, \( \chi_4 = \frac{1}{2} m \langle v_m v_m + j \omega_m \omega_m \rangle \), Eq. (3) is now

\[
\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_i} (\rho e U_i)
\]

\[
= U_m \frac{\partial}{\partial x_i} (\rho e_{jmn} \langle v'_m v'_n \rangle) - \rho \langle v'_m v'_m \rangle \frac{\partial U_m}{\partial x_i}
\]

\[
- \frac{\partial}{\partial x_i} \left( \frac{1}{2} \rho \langle (v'_m v'_m v'_m) + j \langle \omega'_m \omega'_m v'_i \rangle \rangle \right) - \rho j \langle \omega'_m v'_i \rangle \frac{\partial W_m}{\partial x_i},
\]

(13)
or

\[
\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_i} (\rho e U_i) = t_{Curtiss} U_m - t_{Boltzmann} U_{m,i} - q_{i,i} - m_{im} W_{m,i}.
\]

(14)

It should be noted that because of the molecular rotation, the heat flux density has an additional term involving rotation and is now defined as

\[
q_{i,i} = \frac{1}{2} \rho \left( \langle v'_m v'_m v'_i \rangle + j \langle \omega'_m \omega'_n v'_i \rangle \right).
\]

3. Comparison of the Advanced Kinetic and Micropolar Theories for Morphing Continuum

By introducing the kinetic variables into the Boltzmann-Curtiss equation, Eq. 3, the four balance laws can also be found as

\[
\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_i} (\rho U_i) = 0,
\]

\[
\frac{\partial}{\partial t} (\rho U_j) + \frac{\partial}{\partial x_i} (\rho U_i U_j) = -\frac{\partial}{\partial x_i} \left( \rho \langle v'_i v'_j \rangle + \rho c_{jmn} \rho_n \langle \omega'_m \omega'_n \rangle \right),
\]

\[
\frac{\partial}{\partial t} (\rho W_m) + \frac{\partial}{\partial x_i} (\rho j W_m U_i) = -\frac{\partial}{\partial x_i} \left( \rho j \langle \omega'_m v'_i \rangle \right)
\]

\[
\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_i} (\rho e U_i) = \frac{U_m}{m} \frac{\partial}{\partial x_i} \left( \rho c_{jmn} \rho_n \langle \omega'_m v'_j \rangle \right) - \rho j \langle \omega'_m v'_i \rangle \frac{\partial W_m}{\partial x_i} - \frac{1}{2} \rho \left( \langle v'_m v'_m v'_i \rangle + j \langle \omega'_m \omega'_n v'_i \rangle \right) - \rho j \langle \omega'_m v'_i \rangle \frac{\partial W_m}{\partial x_i}.
\]

(15)

3.1. The Zero-order Approximation

If the mean free path is small compared to other characteristic lengths, the system rapidly comes to a local equilibrium. In classical kinetic theory, it is well known that the zero-order approximation reduces the Boltzmann equations to the governing equations for inviscid flow (i.e., Euler equations). Here, the zero-order approximation is applied to the Boltzmann-Curtiss equations (i.e., to Eq. [15]). First assume that the gas has a local Boltzmann-Curtiss distribution, with slowly varying temperature, density, velocity and rotation, so the distribution can be approximated by

\[
\bar{f}(x, v, \omega) \approx f^0(x, v, \omega) = n \left( \frac{m \sqrt{2}}{2 \pi k T} \right)^3 \exp \left[ - \frac{m (v^2 + j \omega^2)}{2k T} \right].
\]

(16)

It should be noted that the Boltzmann-Curtiss distribution is not the exact solution to Eq. [1] however, it serves as a reasonable approximation just as the Maxwell-Boltzmann distribution serves as a good approximation for classical kinetic theory. In the previous section, it has already been shown that \( \langle v'_i v'_i \rangle = 3nkT \) and consequently, the pressure
becomes

\[
\begin{align*}
\tau_{ij}^{\text{Boltzmann},0} &= P_{ij}^0 \\
&= \frac{\rho}{n} \int\int n v_i v_j \left( \frac{m \sqrt{j}}{2\pi k\theta} \right)^3 \exp \left[ -\frac{m(v^2 + j\omega^2)}{2k\theta} \right] d^3v' d^3\omega' \\
&= nk\theta\delta_{ij}.
\end{align*}
\]

(17)

In addition, it is straightforward to prove that

\[
\begin{align*}
t_{ij}^{\text{Curtiss},0} &= \frac{\rho}{n} \varepsilon_{jmn} r_n \int\int n v'_i \omega'_m \left( \frac{m \sqrt{j}}{2\pi k\theta} \right)^3 \exp \left[ -\frac{m(v^2 + j\omega^2)}{2k\theta} \right] d^3v' d^3\omega' = 0, \\
m_{ij}^0 &= \frac{\rho}{n} \int\int n \omega'_m v'_i \left( \frac{m \sqrt{j}}{2\pi k\theta} \right)^3 \exp \left[ -\frac{m(v^2 + j\omega^2)}{2k\theta} \right] d^3v' d^3\omega' = 0, \\
q_i^0 &= \frac{\rho}{2n} \int\int n (v'_m v'_n v'_i + j\omega'_m \omega'_n v'_i) \left( \frac{m \sqrt{j}}{2\pi k\theta} \right)^3 \exp \left[ -\frac{m(v^2 + j\omega^2)}{2k\theta} \right] d^3v' d^3\omega' = 0.
\end{align*}
\]

(18)

With these results, Eqs. (15) reduce to

\[
\begin{align*}
\frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_i} (\rho U_i U_j) &= 0, \\
\frac{\partial}{\partial t} (\rho U_j) + \frac{\partial}{\partial x_i} (\rho U_i U_j) &= -\frac{\partial}{\partial x_i} (nk\theta\delta_{ij}), \\
\frac{\partial}{\partial t} (\rho j W_m) + \frac{\partial}{\partial x_i} (\rho j W_m U_i) &= 0, \\
\frac{\partial}{\partial t} (pe) + \frac{\partial}{\partial x_i} (pe U_i) &= -nk\theta U_{i,i}
\end{align*}
\]

(19)

3.2. Comparison with Eringen’s Micropolar Continuum Theory

Inspired by the Cosserat Brothers, Eringen formulated a micropolar continuum theory for fluid flow containing inner structures [13,14]. With the linear constitutive equations,
the governing equations are found to be
\[
\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho v_i^{\text{MCT}}) = 0,
\]
\[
\frac{\partial}{\partial t}(\rho v_j^{\text{MCT}}) + \frac{\partial}{\partial x_i}(\rho v_j^{\text{MCT}}v_i^{\text{MCT}}) = -p_{,j} + (\lambda + \mu)v_{m,mj}^{\text{MCT}} + (\mu + \kappa)v_{j,mm}^{\text{MCT}} + \kappa e_{jki}\omega_{i,k}^{\text{MCT}},
\]
\[
\frac{\partial}{\partial t}(\rho i_{jk}\omega_k^{\text{MCT}}) + \frac{\partial}{\partial x_i}(\rho i_{jk}\omega_k^{\text{MCT}}v_i^{\text{MCT}}) = (\alpha + \beta)\omega_{m,mj}^{\text{MCT}} + \gamma\omega_{j,mm}^{\text{MCT}} + \kappa (e_{jki}v_{i,k}^{\text{MCT}} - 2\omega_j^{\text{MCT}}),
\]
\[
\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i}(\rho ev_i^{\text{MCT}}) = -p v_{m,m}^{\text{MCT}}.
\] (21)

In comparing Eqs. (19) and (21) it is seen that the equations of MCT and advanced kinetic theory are identical! Kinetic theory, by nature, is a bottom-up theory involving physical conjectures and insights while MCT is a top-down theory involving mathematical rigor. However, both theories lead to the same governing equations for inviscid fluid flow.

4. Conclusion

With the rapid growth of research in nonequilibrium thermodynamics of highly compressible flow with high Mach numbers [30, 31], supersonic/hypersonic turbulence [32] and in micro-/nano-fluidics [33], the traditional kinetic theory, or the classical continuum theory, is in conflict with some of the physics observed in the experiments. One of the major reasons for this conflict is that most molecules are either polyatomic or diatomic possessing not only translational but rotational and vibrational energies. Or the flow itself contains motions from more than one length scale and the subscale motion strongly dominates the macroscale motion as in turbulence. Both the classical bottom-up
kinetic theory and top-down continuum theory consider the system to be composed of volumeless monatomic molecules so the effects of the rotational and vibrational effects in polyatomic or diatomic structures or those of rotational eddies in turbulence are ignored and have to be treated in an ad hoc manner.

As shown here, advanced kinetic theory based on the Boltzmann-Curtiss transport equations can treat the effect of inner structure on the bulk scale phenomena through additional degrees of freedoms in rotation. Rational continuum thermodynamics provides the rigorous mathematics needed for a micropolar continuum theory involving the rotational effect of inner structures. Instead of distinguishing between the advanced kinetic theory and micropolar continuum theory, one can impose the mathematical rigor of rational continuum mechanics on the physical constraints (e.g. entropy principle) and insights (e.g. molecular collision) of the advanced kinetic theory for a complex system of fluid flows.

Although neither dissipative nor viscous effects are included in the current study, an appropriate order approximation on the Boltzmann-Curtiss distribution can shed new physical insights on the material constants of the morphing continuum constitutive equations (i.e., on Eq. 46). The integration of micropolar continuum theory and advanced kinetic theory can serve as an alternative theoretical tool for nonequilibrium aerothermodynamics for turbulence and high Knudsen number flows in any system involving translation and rotation of the particles.

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A Derivation of the Boltzmann-Curtiss Distribution

The derivation presents a systematic approach for the Boltzmann-Curtiss distribution with the Boltzmann principle. Let us assume that a closed system contains a large number \( N \) of distinguishable polyatomic molecules in thermal equilibrium with its surroundings at a temperature \( \theta \) and under constant volume conditions. Let \( \epsilon_i \) denote the \( i \)-th nondegenerate energy level having \( n_i \) molecules, where \( i = 0, 1, 2, 3, \ldots, m \).

The number of microstates, \( W \), is given by

\[
W = \frac{N!}{\sum_{i=0}^{m} n_i !}.
\]  

(22)

It should be noted that \( \sum_{i=0}^{m} n_i = N \). The connection between the statistical mechanical description of the system and the bulk thermodynamic description given by the entropy is expressed in the Boltzmann principle, namely

\[
S = k \ln W,
\]

(23)
where $k$ is the well-known Boltzmann constant.

Substitution of Eq. 22 into Eq. 23 gives

$$S = k \ln W = k \ln \left( \frac{N!}{\sum_{i=0}^{m} n_i!} \right) = k \left[ \ln (N!) - \sum_{i=0}^{m} \ln (n_i!) \right].$$

Now suppose that a small amount of energy $\Delta \epsilon$ is added to the system redistributing the number of molecules in different energy levels. Therefore, the change of entropy between the two different states (before and after the energy injection) can be found and expanded with a Taylor’s Series as

$$\Delta S = k \sum_{i=0}^{m} \left\{ \ln (n_i!) - \ln [(n_i + \Delta n_i)!] \right\}$$

$$= k \sum_{i=0}^{m} \Delta n_i \left[ \ln (n_i) - \ln (n_i + \Delta n_i) \right] + O(\Delta n_i^2)$$

$$\approx k \sum_{i=0}^{m} \Delta n_i \ln \left( \frac{n_i}{n_i + \Delta n_i} \right). \quad (24)$$

From the laws of thermodynamics, the connection between the entropy $S$ and total energy $U$ of the system is $dS = dU/\theta$. Consequently,

$$\Delta S = \int dS = \int \frac{dU}{\theta} = \frac{1}{\theta} \int dU = \frac{1}{\theta} \Delta U. \quad (25)$$

With the assumption that temperature remains effectively constant, the energy change $\Delta U$ is the energy $\Delta \epsilon = \frac{1}{2} m (\Delta v^2 + j \Delta \omega^2)$ injected into the original system. As a result, Eq. 25 becomes

$$\Delta S = \frac{1}{\theta} \Delta \epsilon = \frac{1}{2\theta} \Delta (v^2 + j \omega^2). \quad (26)$$

Combine Eqs. 24 and 26 to obtain

$$k \sum_{i=0}^{m} \Delta n_i \ln \left( \frac{n_i}{n_i + \Delta n_i} \right) = \frac{1}{2\theta} m (\Delta v^2 + j \Delta \omega^2),$$

or, equivalently,

$$\sum_{i=0}^{m} \left( \frac{n_i + \Delta n_i}{n_i} \right)^{\Delta n_i} = \exp \left[ -\frac{1}{2k\theta} m (\Delta v^2 + j \Delta \omega^2) \right]. \quad (27)$$

Equation 27 is the Boltzmann–Curtiss distribution (c.f. eq. 4) used for the Boltzmann–Curtiss transport equations and is the basis of the morphing continuum theory at equilibrium.
B Rational Continuum Thermomechanics for Micropolar Theory

A morphing continuum is a collection of continuously distributed, oriented, finite-size particles that can rotate. A material point $P$ in the reference frame is identified by a position and three directors attached to the material point.

The motion, at time $t$, carries the finite-size particle to a spatial point and rotates the three directors to a new direction. Thus, such a motion is similar to the motion of a liquid molecule approximated as a sphere. It has not only translational velocity, but also self-spinning gyration on its own axis. These motions and their inverse motions for the morphing continuum can be described as

$$
x_k = x_k(X_K, t) \quad \quad \quad X_K = X_K(x_k, t)
\xi_k = \chi_{kK}(X_K, t) \Xi_K \quad \quad \quad \Xi_K = \chi_{KK} \xi_k
K = 1, 2, 3 \quad \quad \quad k = 1, 2, 3
$$

and

$$
\chi_{kK} \chi_{lK} = \delta_{kl} \quad \quad \quad \tilde{\chi}_{kK} \tilde{\chi}_{lk} = \delta_{KL}.
$$

It is straightforward to prove that

$$
\chi_{kK} = \tilde{\chi}_{kK}.
$$

Consequently, the right-hand part of Eq. 29 becomes

$$
\chi_{kK} \chi_{kL} = \delta_{KL}.
$$

Here and throughout, an index followed by a comma denotes a partial derivative, e.g.,

$$
x_{k,K} = \frac{\partial x_k}{\partial X_K} \quad \quad \quad \quad X_{K,k} = \frac{\partial X_K}{\partial x_k}.
$$

For fluid flow, deformation-rate tensors are used to characterize the viscous resistance. Deformation-rate tensors may be deduced by calculating the material time derivative of the spatial deformation tensors. For the morphing continuum, two objective deformation-rate tensors are

$$
a_{kl} = v_{l,k}^{\text{MCT}} + e_{likm} \omega_{m}^{\text{MCT}} \quad \quad \quad b_{kl} = \omega_{k,l}^{\text{MCT}},
$$

where $v_{k}^{\text{MCT}}$ is the velocity vector and $\omega_{k}^{\text{MCT}}$ is the self-spinning gyration vector. If a fluid molecule is assumed to be a rigid body particle, it possesses two types of motion, translational velocity ($v_{k}^{\text{MCT}}$), found by solving the MCT linear momentum equation, and spinning gyration ($\omega_{k}^{\text{MCT}}$) found by solving the MCT angular momentum equation. In the classical Navier-Stokes equations, only the translational velocity can be directly solved from the balance law of linear momentum. To investigate the effect of the rotational motion of the molecule, one must use the velocity field and take the angular velocity to be one-half of the vorticity i.e., $\frac{1}{2}e_{ijk} v_{j,i}^{\text{MCT}}$. This approximation in the Navier-Stokes
equations limits not only predicting the flow physics involving molecular spinning, but also fails to represent the interaction between translation and spinning.

Thermodynamic balance laws for morphing continuum theory include (1) conservation of mass; (2) conservation of linear momentum; (3) conservation of angular momentum; (4) conservation of energy; and (5) the Clausius-Duhem inequality. All five can be expressed as follows:

**Balance Law of mass**

\[ \frac{\partial \rho}{\partial t} + (\rho \nu_{i,i}^{\text{MCT}}) = 0 \]  

**Balance Law of linear momentum**

\[ t_{lk,l} + \rho (f_k - \dot{\omega}_k^{\text{MCT}}) = 0 \]  

**Balance Law of angular momentum**

\[ m_{lk,l} + \epsilon_{ijk} t_{ij} + \rho i_{km} (l_m - \dot{\omega}_m^{\text{MCT}}) = 0 \]  

**Balance Law of energy**

\[ \rho \dot{e} - t_{kl} a_{kl} - m_{kl} b_{lk} + q_{k,k} = 0 \]  

**Clausius-Duhem inequality**

\[ \rho \left( \dot{\psi} + \eta \dot{\theta} \right) + t_{kl} a_{kl} + m_{kl} b_{lk} - \frac{q_{k,k}}{\rho} \geq 0 \]  

where \( \rho \) is mass density, \( i_{km} \) the microinertia for the shape of the microstructure, \( f_k \) the body force density, \( l_m \) the body moment density, \( \epsilon \) the internal energy density, \( \eta \) the entropy density, \( \psi = e - \theta \eta \) the Helmholtz free energy, \( t_{lk} \) the Cauchy stress, \( m_{lk} \) the moment of stress, and \( q_k \) the heat flux. It is worthwhile to mention that \( t_{lk}, m_{lk} \) and \( q_k \) are the constitutive equations for the morphing continuum theory and can be derived from the Clausius-Duhem inequality (see Eq. 38) through the Coleman-Noll procedure \[7, 11\].

The concept of microinertia, \( i_{km} \equiv \int \rho' \xi_k \xi_m dv' / \int \rho' dv' \equiv \langle \xi_k \xi_m \rangle \), is similar to the moment of inertia in rigid body rotation and measures the resistance of the microstructure to changes to its rotation. It can be further expressed as

\[ j_{km} = i_{pp} \delta_{km} - i_{km} \quad \text{where} \quad j \equiv \frac{1}{3} j_{pp}. \]  

The volume \( v' \) refers to the volume of the finite-size microstructure. If the finite-size particle is assumed to be a solid sphere with a radius \( d \) and a constant density \( \rho \), the microinertia can be computed as \( j = \frac{2}{5} d^2 \). This result shows the microinertia for a spherical microstructure is the moment of inertia of a sphere divided by its mass. The experimental data of Lagrangian velocities of a trace particle can be used to determine the geometry of the microstructure \[34, 35\].
There are multiple different definitions for fluids, including (1) fluids do not have a preferred shape \[36\], and (2), fluids cannot withstand shearing forces, however small, without sustained motion \[37\]. Nevertheless, all these definitions describe the physics of fluid flow, and yet provide little help in mathematically formulating a continuum theory for fluids. In rational continuum thermomechanics, Eringen \[3\] formally defined fluids by saying that “a body is called fluid if every configuration of the body leaving density unchanged can be taken as the reference configuration.”

This definition implies \( x_{k,K} \to \delta_{kK} \) and \( \chi_{kK} \to \delta_{kK} \) where \( \delta_{kK} \) is the shifter, the directional cosine between the current configuration and reference configuration. Hence, the difference between the reference configuration and the current configuration is just a coordinate transformation. As a result, the axiom of objectivity should always be considered and obeyed. The axiom of objectivity, or frame-indifference, states that the constitutive equations must be form-invariant with respect to rigid body motions of the spatial frame of reference \[2, 3\].

The state of fluids in morphing continuum theory is expressed by the characterization of the response functions \( Y = \{ \psi, \eta, t_{kl}, m_{kl}, q_k \} \) as functions of a set of independent variables \( Z = \{ \rho^{-1}, \theta, \theta_k, a_{kl}, b_{lk} \} \). In addition, following the axiom of equipresence, at the outset the constitutive relations are written as \( Y = Y(Z) \).

The Clausius-Duhem inequality of Eq. 38, also known as the thermodynamic second law, is a statement concerning the irreversibility of natural processes, especially when energy dissipation is involved. Feynman et. al. stated “so we see that a substance must be limited in a certain way; one cannot make up anything he wants; ... This [entropy] principle, this limitation, is the only rule that comes out of thermodynamics.” \[38\] After the Coleman-Noll procedure, i.e., combining the inequality with the response function and the independent variables, Eq. 38 reduces to

\[
t_{kl}a_{kl} + m_{kl}b_{lk} - \frac{q_k\theta_k}{\theta} \geq 0. \tag{40}
\]

There are three pairs of thermodynamic conjugates, \((t_{kl}, a_{kl})\), \((m_{kl}, b_{lk})\), and \((\frac{q_k}{\theta}, \theta_k)\) that contribute to the irreversibility of the material. A set of the thermodynamic fluxes \( J \) is defined as \( J = \{ t_{kl}, m_{kl}, \frac{q_k}{\theta} \} \) and are functions of a set of the thermodynamic forces \( (Z^D) \) and other independent variables \( (Z^R) \), \( Z = \{ Z^R; Z^D \} = \{ \rho^{-1}, \theta; a_{kl}, b_{lk}, \theta_k \} \). With these sets of thermodynamic fluxes and thermodynamic forces, the Clausius-Duhem inequality can be rewritten as

\[
J (Z^R; Z^D) \cdot Z^D \geq 0. \tag{41}
\]

Onsager and Edelen proposed that the thermodynamic fluxes can be obtained by the general dissipative function \[6, 39–41\]

\[
J = \frac{\partial \Psi (Z^R, Z^D)}{\partial Z^D} + U, \tag{42}
\]

where the vector-valued function \( U \) is the constitutive residual with \( Z^D \cdot U = 0 \). This result indicates that \( U \) does not contribute to the dissipative or entropy production. For simplicity, one can further set \( U = 0 \).
To determine thermodynamic fluxes for a fluid using the derivative of $\Psi$ with respect to the thermodynamic forces $Z_D$, $\Psi$ needs to be invariant under superimposed rigid body motion, i.e., the dissipative function $\Psi$ must satisfy the axiom of objectivity \cite{6}. Hence, $\Psi$ is an isotropic function of scalar and can be expressed by Wang’s representation theorem \cite{42, 43} as

$$
\Psi\{Z^R, Z^D\} = \Psi\{I_1, I_2, I_3, ..., I_n\} \quad \text{and} \quad J = \frac{\partial \Psi}{\partial Z^D} = \sum_{i=1}^{n} \frac{\partial \Psi}{\partial I_i} \frac{\partial I_i}{\partial Z^D}.
$$

(43)

It should be noted here that $b_{kl}$ and $m_{kl}$ are pseudo-tensors while the rest, including $\theta_k, t_{kl}, q_k$ and $a_{kl}$ are normal tensors \cite{7}. Considering the mixing of pseudo-tensors and normal tensors in $Z^R$ and $Z^D$ for linear constitutive equations, the set of invariants includes $I_1 = a_{(ij)}, I_2 = a_{(ij)}a_{(ji)}, I_3 = b_{(ij)}b_{(ji)}, I_4 = \theta_{k}a_{kl}, I_5 = a_{ij}(a_{ji}), I_6 = b_{ij}b_{ji}$, and $I_7 = e_{ijk}b_{ij}\theta_k$. Here (...) refers to the symmetric part, [...] indicates the anti-symmetric part and $e_{ijk}$ is the permutation symbol. Hence, the thermodynamic fluxes can be further derived as

$$
\begin{align*}
t_{kl} &= t_{(kl)} + t_{[kl]} = \frac{\partial \Psi}{\partial a_{(kl)}} + \frac{\partial \Psi}{\partial a_{[kl]}} = \frac{\partial \Psi}{\partial I_1} \delta_{kl} + \frac{\partial \Psi}{\partial I_2} a_{(kl)} + \frac{\partial \Psi}{\partial I_3} a_{[kl]} \\
m_{kl} &= m_{(kl)} + m_{[kl]} = \frac{\partial \Psi}{\partial b_{(kl)}} + \frac{\partial \Psi}{\partial b_{[kl]}} = \frac{\partial \Psi}{\partial I_4} b_{(kl)} + \frac{\partial \Psi}{\partial I_5} b_{[kl]} + \frac{\partial \Psi}{\partial I_7} e_{klm}\theta_{,m} \\
q_k &= \frac{\partial \Psi}{\partial \theta_k} = \frac{\partial \Psi}{\partial I_4} \theta_k + \frac{\partial \Psi}{\partial I_7} e_{ijk}b_{ij}
\end{align*}
$$

(44)

These equations can also be put into matrix form as

$$
\begin{bmatrix}
t_{(kl)} \\
t_{[kl]} \\
m_{(kl)} \\
m_{[kl]} \\
q_k
\end{bmatrix} = \begin{bmatrix}
\lambda\delta_{kl} + 2\mu + \kappa & 0 & 0 & 0 & 0 \\
0 & \kappa & 0 & 0 & 0 \\
0 & 0 & \alpha\delta_{kl} + \frac{1}{2}(\beta + \gamma) & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2}(\beta - \gamma) & \frac{\alpha\epsilon_{klm}}{\kappa} \\
0 & 0 & 0 & 0 & \theta_{,m}
\end{bmatrix}\begin{bmatrix}
a_{(kl)} \\
a_{[kl]} \\
b_{(kl)} \\
b_{[kl]} \\
\theta_{,m}
\end{bmatrix}.
$$

(45)

Notice the symmetry of this thermodynamic matrix. Equations \cite{44, 45} connect the thermodynamic fluxes and the thermodynamic forces, and can be referred to as Onsager’s reciprocal relations derived in 1931 \cite{40, 41} leading to his Nobel Prize in Chemistry in 1968. With further algebraic manipulation, the linear constitutive equations for the morphing continuum are

$$
\begin{align*}
t_{kl} &= -p\delta_{kl} + \lambda a_{m,m}^{\text{MCT}}\delta_{kl} + (\mu + \kappa) \left( e_{l,k}^{\text{MCT}} + e_{lkm}\omega_{m}^{\text{MCT}} \right) + \mu \left( e_{l,k}^{\text{MCT}} + e_{lkm}\omega_{m}^{\text{MCT}} \right) \\
m_{kl} &= \frac{\alpha\tau}{\theta} e_{klm}\theta_{,m} + \alpha\omega_{m,m}^{\text{MCT}}\delta_{kl} + \beta\omega_{k,l}^{\text{MCT}} + \gamma\omega_{l,k}^{\text{MCT}} \\
q_k &= \frac{\alpha\tau}{\theta} e_{klm}\omega_{k,l}^{\text{MCT}} + K\theta_{,m}
\end{align*}
$$

(46)

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