The Effect of Kinetic Energies on the Relationship Between Molecular Collision Speed and Acoustic Wave Speed

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Abstract

Acoustic waves are the result of molecules colliding and fluctuating. However, the relationship between acoustic wave speed and molecular collision speed has not been directly formulated and validated as a function of kinetic properties in terms of the translational and rotational kinetic energies. This article will present and validate a formula that connects acoustic wave speed and molecular collision speed with the translational and rotational kinetic energies of molecules. This formula not only provides insight into the microscopic mechanisms of acoustic waves but can also be used to determine acoustic wave speed from mechanic analyses such as collision simulations of particles.

Keywords: acoustic wave speed, molecular collision speed, the ratio of heat capacity, heat capacity at constant pressure, heat capacity at constant volume, kinetic theory of gases, kinetic energy.

Introduction

Acoustic waves are the result of molecules colliding and fluctuating [1,2]. However, the relationship between acoustic wave speed and molecular collision speed has not been directly formulated and validated as a function of kinetic properties in terms of the translational and rotational kinetic energies of molecules. The author[1] and his co-authors have documented a formula for this purpose in a published lecture notes [3] without a self-contained proof of this formula. In this article, this formula will be derived in detail based only on mechanical properties.

The relationship between molecular collision speed (v) and acoustic wave speed (c) is typically formulated as [2]

$$c^2 = \frac{\gamma}{3} v^2 \tag{1}$$

Where γ is the ratio of heat capacity [1,4] defined as the ratio of the heat capacity at constant pressure (C_P) to the heat capacity at constant volume (C_V) as

$$\gamma \equiv \frac{C_P}{C_V} \tag{2}$$

The ratios of heat capacity (γ) for different molecules are obtained experimentally. Kinetic energies, in terms of the translational and rotational kinetic energies, are not shown explicitly in the formulas.

We propose a new formula for the ratio of heat capacity that relates the molecular collision speed (v) with the acoustic wave speed (c) as

$$\gamma = \frac{3\alpha+2}{3\alpha} \tag{3}$$

where α is a new variable defined as the ratio of total kinetic energy ($E_t + E_r$) to translational kinetic (E_r) energy as

$$\alpha \equiv \frac{E_t+E_r}{E_t} \tag{4}$$

Where E_t is the translational kinetic energy, E_r is the rotational (spin) kinetic energy, and $E_t + E_r$ is the total kinetic energy.

From the new proposed ratio of heat capacity formula (Eq.3), the relationship between the molecular collision speed (v) and the acoustic wave speed (c) is affected by the ratio of kinetic energies in terms of the new variable α as shown in Eq.1.

The resulting formula from combining the above three equations (Eqs.1,3,4) connects acoustic wave speed and molecular collision speed with the translational and rotational kinetic energies of molecules. This formula provides insight into the microscopic mechanisms of acoustic waves. In a practical sense, the wave speed can be determined from mechanic analyses such as collision simulations of particles.

This new proposed formula (Eq.3) with the new variable α (Eq.4) will be derived as following: First, we will derive the equation of state which is defined with the new variable α. Second, we will derive the acoustic wave equation using equation of state with the new variable α. Third, we will derive the formula (Eq.1) that relates the molecular collision speed (v) to the wave propagation speed (c).

Three Governing Equations

To derive the acoustic wave equation, three governing equations are required: the equation of state, Euler's force equation, and the equation of continuity. These three governing equations connect three physical properties: pressure (P), collision velocity (v), and density (ρ) as shown in the figure below.

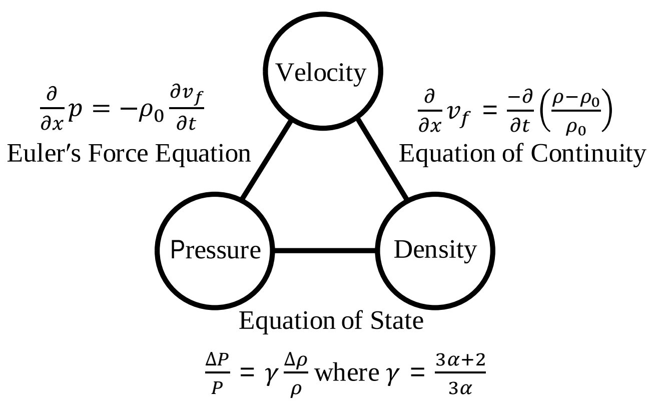

Figure 1. Three Governing Equations

The equation of state will be derived in detail using the new formula for the ratio of heat capacity (γ). Euler's force equation and the equation of continuity will be briefly derived as they are well documented in literature.

Equation of State

To setup the derivation of the equation of state, three equations (Eqs. 5-7) based on the kinetic theory are listed below for reference:

$$E_t = \frac{1}{2} n N_A m v^2 \tag{5}$$

$$E_r = \frac{1}{2} n N_A I \omega^2 \tag{6}$$

$$PV = \frac{1}{3} n N_A m v^2 \tag{7}$$

where E_t is the translational kinetic energy, E_r is the rotational kinetic energy, n is the number of moles, N_A is Avogadro's number, m is the mass of one molecule, I is the mass moment of inertia of one molecule, v is the translational velocity, ω is the angular velocity, P is the pressure, and V is the volume.

Combining Eqs.5 and 7, the translational kinetic energy E_t can be related to the pressure P as

$$E_t = \frac{3}{2} PV \tag{8}$$

This equation (Eq.8) shows that at a fixed volume (V), pressure (P) is only related to the translational kinetic energy (E_t) and is not related to the rotational kinetic energy (E_r). This is an important property for the kinetic theory of gases which will be used to develop the formula for the equation of state as following.

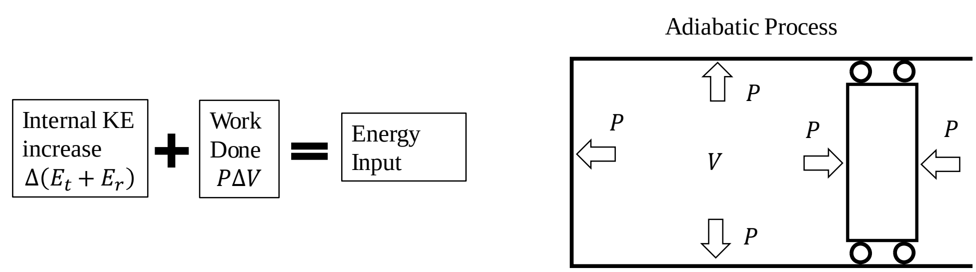

Figure 2. Adiabatic Process

The equation of state in terms of the translational kinetic energy (E_t) and the rotational kinetic energy (E_r) is derived as following. In an adiabatic process, according to the conservation of energy, if there is no energy input ($\Delta Q = 0$), the summation of the change in internal kinetic energy ($\Delta E_t + \Delta E_r$) and the work done ($P\Delta V$) is equal to zero as

$$\Delta(E_t + E_r) + P\Delta V = 0 \tag{9}$$

Since pressure (P) is only related to the translational kinetic energy (E_t) and not to the rotational kinetic energy (E_r) as shown in Eq.8, we want to represent the total kinetic energy increase ($\Delta E_t + \Delta E_r$) with the translational kinetic energy increase (E_t). This is accomplished by introducing a new variable α defined as the ratio of the total kinetic energy ($E_t + E_r$) to the translational kinetic energy (E_t) as

$$\alpha \equiv \frac{E_t + E_r}{E_t} \tag{10}$$

Substituting Eq.10 into Eq.9 gives

$$\Delta(\alpha E_t) + P\Delta V = 0 \tag{11}$$

Substituting Eq.8 into the above equation (Eq 11) gives

$$\alpha \frac{3}{2}\Delta(PV) + P\Delta V = 0 \tag{12}$$

Taking the derivative of PV gives

$$\alpha \frac{3}{2}(\Delta P \cdot V + P \cdot \Delta V) + P\Delta V = 0 \tag{13}$$

Rearrangement of the above equation gives the equation of state that relates pressure change to volume change of the transmission media as

$$\frac{\Delta P}{P} = -\left(\frac{3\alpha+2}{3\alpha}\right)\frac{\Delta V}{V} \tag{14}$$

According to the conservation of mass, $\Delta m = \Delta(\rho V) = 0$, volume change ($\frac{\Delta V}{V}$) is related to density change ($\frac{\Delta \rho}{\rho}$) as

$$\frac{\Delta V}{V} = -\frac{\Delta \rho}{\rho} \tag{15}$$

Substituting Eq.15 into Eq.14 gives the equation of state as

$$\frac{\Delta P}{P} = \gamma \frac{\Delta \rho}{\rho} \tag{16}$$

Where $\frac{3\alpha+2}{3\alpha}$ is the ratio of heat capacity (γ) as

$$\gamma = \frac{3\alpha+2}{3\alpha} \tag{17}$$

For monatomic gases with $E_r = 0$, $\alpha = 1$, $\gamma = \frac{5}{3}$. For diatomic gases with $E_r = \frac{2}{3}E_t$, $\alpha = \frac{5}{3}$, $\gamma = \frac{7}{5}$.

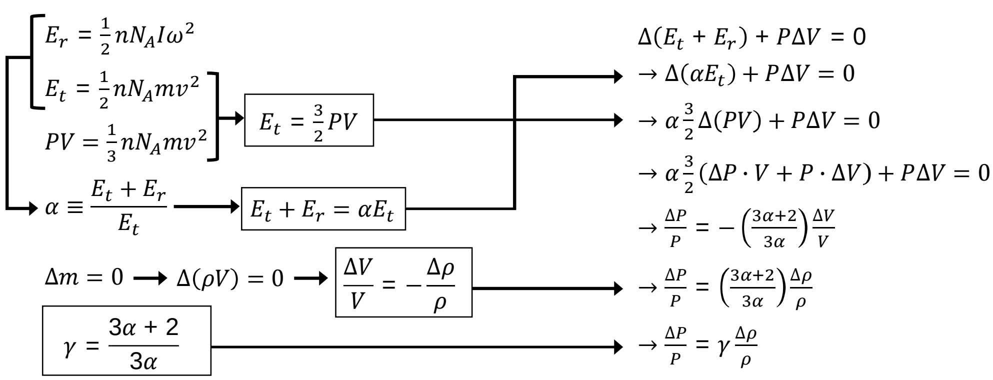

Figure 3. Flowchart of the Derivation of the Equation of State

The Euler's Force Equation

The Euler's force equation can be derived from Newton's second law of motion. According to Newton's Law of Motion, the force $\vec{f}$ applied on the cubic will cause an acceleration $\vec{a}$ on this cubic with three-dimensional lengths of Δx, Δy, $and\ \Delta z$. The free body diagram of the cubic is shown in the figure below.

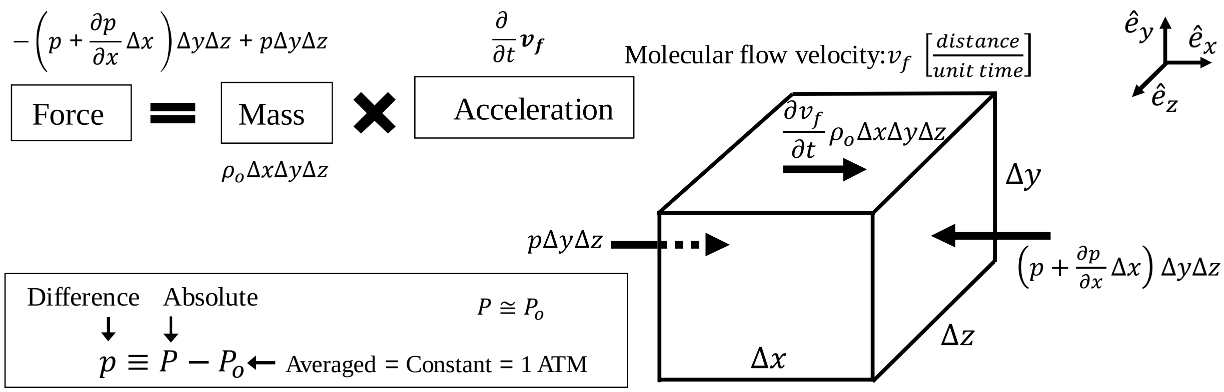

Figure 4. Newton's Second Law of Motion

The governing equation of the cubic can be expressed as:

$$-\left(p+\frac{\partial p}{\partial x}\cdot\Delta x\right)\Delta y\Delta z+(p)\Delta y\Delta z=\rho_0\Delta x\Delta y\Delta z\cdot\frac{\partial}{\partial t}v_f \tag{18}$$

Simplifying the equation above by eliminating $\Delta x\Delta y\Delta z$ yields the one-dimensional Euler's force equation in Cartesian coordinates:

$$\frac{\partial p}{\partial x}=-\rho_o\frac{\partial}{\partial t}v_f \tag{19}$$

Where $p\equiv P-P_o$ and $P\cong P_o$. Here P is the instantaneous pressure and P_o is the averaged pressure which can be treated as a constant. Based on this, Eq.16 can be rewritten as

$$\frac{P-P_o}{P_o}=\gamma\frac{\rho-\rho_o}{\rho_o} \tag{20}$$

Note that ρ is the instantaneous density and ρ_o is the averaged density and can be treated as a constant.

Equation of Continuity

The equation of continuity can be derived from the law of conservation of mass. According to the law of conservation of mass, the increase of mass in the cubic unit is equal to the "mass flow in" minus "mass flow out", as shown in the figure below:

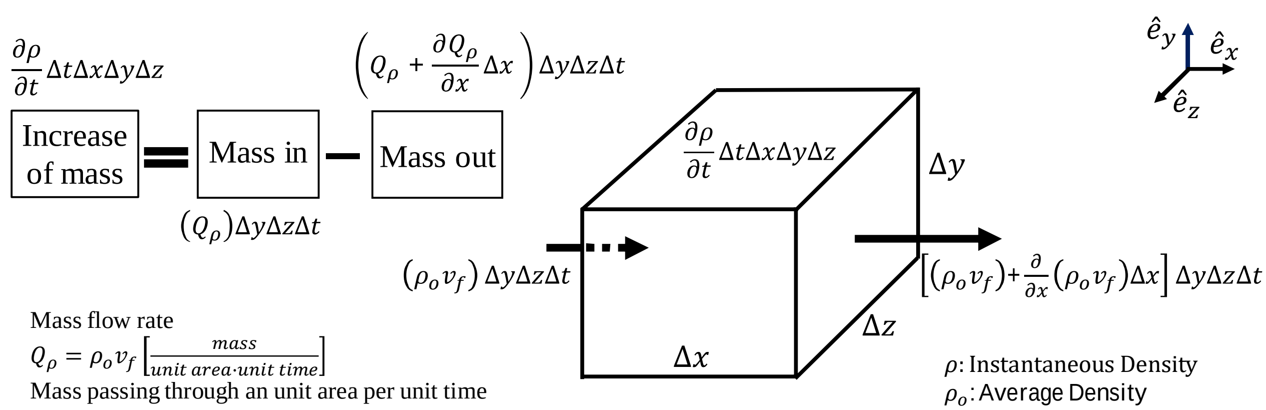

Figure 5. Equation of Continuity

The governing equation of the cubic can be expressed as:

$$\frac{\partial \rho}{\partial t} \cdot \Delta t \cdot \Delta x \Delta y \Delta z = Q_\rho \cdot \Delta y \Delta z \cdot \Delta t - \left(Q_\rho + \frac{\partial Q_\rho}{\partial x} \Delta x\right) \cdot \Delta y \Delta z \cdot \Delta t \qquad (21)$$

Where Q_ρ is the mass flow rate defined as $\rho_o v_f$. The above equation can be simplified to the one-dimensional equation of continuity in Cartesian coordinates as:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}\left(\rho_o v_f\right) \qquad (22)$$

Since ρ is the instantaneous density and ρ_o is the averaged density which can be treated as a constant, therefore $\partial \rho \equiv \partial(\rho - \rho_o)$. The equation above (Eq.22) can be rewritten as

$$\frac{\partial v_f}{\partial x} = -\frac{\partial}{\partial t}\left(\frac{\rho - \rho_o}{\rho_o}\right) \qquad (23)$$

Acoustic Wave Equation

Finally, the acoustic wave equation can be obtained by combining the three governing Eqs.19,20,23 to get

$$\frac{\partial^2}{\partial x^2} p(x,t) = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} p(x,t) \qquad (24)$$

where

$$c^2 = \frac{\gamma P_o}{\rho_o} \qquad (25)$$

Where c is the speed of sound, P_o is the averaged pressure, and ρ_o is the averaged density.

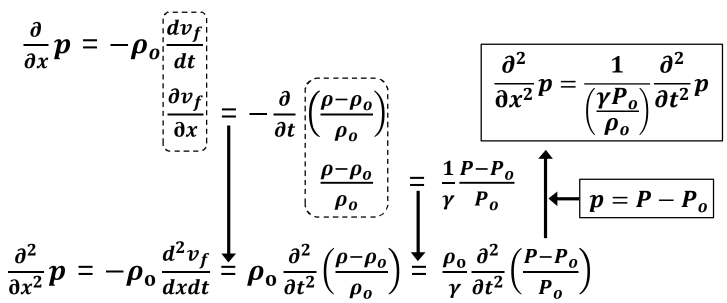

Figure 6. Derivation of the Acoustic Wave Equation

The relationship between the wave propagation speed (c) and the molecular collision speed (v) can be obtained by replacing the pressure (P_o) with $\frac{1}{3V} n N_A m v^2$ as shown in Eq.7 and replacing density (ρ_o) with $\frac{n N_A m}{V}$ as

$$c^2 = \frac{\gamma P_o}{\rho_o} = \frac{\gamma \frac{1}{3V} n N_A m v^2}{\frac{n N_A m}{V}} = \frac{\gamma}{3} v^2 \qquad (26)$$

Where γ is the ratio of heat capacity defined as

$$\gamma = \frac{3\alpha + 2}{3\alpha} \qquad (27)$$

where α is the new variable defined as the ratio of total kinetic energy ($E_t + E_r$) to translational kinetic (E_r) energy as

$$\alpha \equiv \frac{E_t+E_r}{E_t} \tag{28}$$

Where E_t is the translational kinetic energy, E_r is the rotational kinetic energy, and $E_t + E_r$ is the total kinetic energy.

The relationship between acoustic wave speed and molecular collision speed (Eqs.1 or 26) is now validated with the translational and rotational kinetic energies of molecules (Eqs.5 and 6). The relationship between acoustic wave speed and molecular collision speed is affected by the kinetic energies as following: when the rotational kinetic energy (E_r) is very small relative to the translational kinetic energy (E_t), the ratio of heat capacity (γ) will be close to 5/3 and the acoustic wave speed (c) will be close to the molecular collision speed (v) multiplied by $\sqrt{\frac{5}{9}}$ as shown in Eq.26. On the other hand, when the rotational kinetic energy (E_r) is very large relative to the translational kinetic energy (E_t), the ratio of heat capacity (γ) will be close to 1 and the acoustic wave speed (c) will be close to the molecular collision speed (v) multiplied by $\sqrt{\frac{1}{3}}$. By comparing these two extreme cases, if the molecular collision speed (v) is fixed, the acoustic wave speed (c) is faster in particles with smaller rotational energies and slower in particle with larger rotational energies. This can be explained by the derivation that rotational energy absorbs part of the kinetic energy and hence slows down the acoustic wave speed.

Conclusion

A formula that connects acoustic wave speed and molecular collision speed with kinetic properties in terms of the translational and rotational kinetic energies is presented and validated based only on kinetic properties. This formula not only provides insight into the acoustic microscopic mechanisms of acoustic waves but also can be used to determine the wave speed from the mechanic analysis such as the numerical collision simulation of particles.

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