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Recent Advances in the Analysis and Simulation of Compressible Flow Problems: The 75th Anniversary of the Landmark Report by Lagerstrom, Cole, & Trilling (1949)

A Lagrangian for Compressible Flow Focusing on Dissipation due to Thermal Conduction

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ABSTRACT

With the aim of describing compressible viscous flows by means of a variational principle that takes into account heat conduction, a recently proposed Lagrangian is subjected to a detailed linear wave analysis that stems directly from the Lagrangian. The accompanying thermodynamic equation of state employed leads to a natural decomposition of the conduction term into three contributions, with the importance of each accessed through a detailed analysis employing a recently developed perturbation methodology giving rise to a favorable system of governing Jacobi equations. In addition to the model Lagrangian itself, three potential model scenarios—based on different combinations of the contributions forming the Lagrangian—are rigorously evaluated and appraised, regarding the occurrence, or otherwise, of dissipation recognizable by an attenuation of harmonic waves. Results reveal that two of the four models are suitable candidates, and suggest one in particular.

1 | Introduction

Classical Lagrange formalism has its origins in the developments of the 18th century, being subsequently rebadged analytical mechanics following Hamilton in the 19th century, where the research focus was purely on conservative mechanical systems and the Lagrangian was strictly defined as the difference of kinetic and potential energy. This remains the current standing as evidenced in recent standard textbooks [1]. However, beginning with the 20th century, serious research began to extend the concept of variational principles to *dissipative systems*, beginning with Bateman's early work [2] and later advancements reported, for example, by Vujanovic and Jones [3], where variational formulations for heat transfer in incompressible flows, of a boundary layer type and non-Newtonian nature, are proposed using the method of vanishing parameters. Later, Anthony [4, 5] formulated a detailed construct of the thermodynamics of irreversible processes taking thermal degrees of freedom into consideration, such that the total energy[1] is still conserved according to Noether's theorem, while including dissipation in the wider sense of an irreversible transfer of mechanical energy (kinetic energy) to thermal (inner) energy.

More recently, a rigorous analysis of Galilean symmetry and associated Noether densities and fluxes, by Scholle [6], established a general scheme for Lagrangians, providing in addition a deeper justification for the representation of the velocity field in terms of Clebsch variables [7–10]. In this context, it is shown that Seliger and Whitham's Lagrangian [11] for inviscid flow, being undoubtedly a milestone in the field of fluid dynamics employing

Abbreviations: ATM, all-terms model; CM, continuous model; LES, linear equation set; MM, minimalistic model; RDM, reduced discontinuous model.

variational methods, accords with the above. Another essence of Seliger and Whitham's work (and similar earlier work of Lin [12]) is the use of another potential field ϑ fulfilling:

$$\left\{\partial_t + \vec{u} \cdot \nabla\right\}\vartheta = T, \tag{1}$$

where T denotes temperature. This additional thermal degree of freedom is frequently referred as *thermasy* [13] or *thermal displacement* [14–16].

As an advancement of Seliger and Whitham's work [11], the Lagrangian of Zuckerwar and Ash [17] includes volume viscosity and therefore dissipation. However, the price for this is the occurrence of a nonclassical feedback of the thermasy/thermal displacement ϑ to the flow [18, 19] that cannot be understood within the framework of conventional thermodynamics with the assumption of a local equilibrium.

By reformulating the two thermal degrees of freedom occurring in Zuckerwar and Ash's Lagrangian, the specific entropy s and the thermasy/thermal displacement in terms of Anthony's *thermal excitation* [4, 5, 20] as

$$\chi = \sqrt{c_0 T_0}\exp\left(\frac{s}{2c_0} - \mathrm{i}\omega_0 \exp\left(-\frac{s}{c_0}\right)\frac{\vartheta}{T_0}\right), \tag{2}$$

with an additional parameter ω_0 occurring alongside the reference values $c_0 = c_V(\varrho_0, T_0)$ and T_0 for specific heat and temperature, respectively, the above issue can be addressed by reducing the nonclassical feedback terms to order ω_0^{-1}; whereby discontinuities inevitably occur due to the logarithm of the thermal excitation [21]. On eliminating the discontinuities by time, or ensemble, averaging [22, 23] the nonclassical contributions are reduced to order ω_0^{-2}. In this context, the parameter ω_0 can be interpreted as a relaxation rate toward thermodynamic equilibrium. Further advancements relating to shear viscosity and heat conduction have also been reached in the aforementioned papers.

In contrast to the above, the work reported here focuses on thermal conduction and its crucial role in dissipative processes in compressible flow. In Section 2 the Lagrangian proposed in previous work [23] is considered with regard to a particular thermodynamic equation of state, leading naturally to a decomposition of the heat conduction term into three parts. To assess the impact of each of these three contributions on the system, a recently established variational perturbation approach [24] is applied in Section 3, resulting in a system of linearized evolution equations for small perturbations to the rest state. Obtaining solutions in the form of harmonic waves, a dispersion relation results which is carefully analyzed for four different scenarios regarding the heat conduction component of the Lagrangian considering: (i) only the leading term as proposed in prior work [23]; (ii) neglect of the discontinuous term; (iii) the leading and the discontinuous term; and (iv) all terms. In the discussion which follows, Section 4, attention is directed to dissipation, that is, the irreversible transfer of kinetic energy to inner energy and, in particular, the role of the discontinuous term with respect to the latter. In Section 5, conclusions are drawn and future research avenues discussed.

2 | Modeling Approach

2.1 | Proposed Lagrangian

2.1.1 | General Lagrangian Considering Both Viscosity and Thermal Conduction

For the compressible viscous flow of a Newtonian fluid with thermal conduction, the following Lagrangian [23] is proposed in terms of the density ϱ, the Clebsch variables φ, α, ξ, the velocity $\vec{u}$, and the thermal excitation χ, which can be conveniently subdivided into three parts:

$$\ell = \ell_{\text{rev}} + \ell_{\text{visc}} + \ell_{\text{cond}}, \tag{3}$$

$$\ell_{\text{rev}} = -\varrho\left[\left\{\partial_t + \vec{u}\cdot\nabla\right\}\varphi + \alpha\left\{\partial_t + \vec{u}\cdot\nabla\right\}\xi + \frac{1}{\omega_0}\mathfrak{I}\left(\bar{\chi}\left\{\partial_t + \vec{u}\cdot\nabla\right\}\chi\right) - \frac{\vec{u}^2}{2} + e\right], \tag{4}$$

$$\ell_{\text{visc}} = \frac{1}{\mathrm{i}\omega_0}\ln\sqrt{\frac{\bar{\chi}}{\chi}}\left[\frac{\eta}{4}\mathrm{tr}\left[\nabla\otimes\vec{u} + \left(\nabla\otimes\vec{u}\right)^t\right]^2 + \frac{\eta'}{2}\left(\nabla\cdot\vec{u}\right)^2\right], \tag{5}$$

$$\ell_{\text{cond}} = -\lambda\nabla T\cdot\nabla\left(\frac{\vartheta}{T}\right) = -\frac{\lambda}{\mathrm{i}\omega_0 c_0}\nabla\mathfrak{R}\left(\chi\frac{\partial e}{\partial\chi}\right)\cdot\nabla\left(\frac{\bar{\chi}\chi\ln\sqrt{\bar{\chi}/\chi}}{\mathfrak{R}(\chi\partial e/\partial\chi)}\right); \tag{6}$$

a *reversible* part, ℓ_{rev}, for an inviscid flow without thermal conduction equivalent to the classical Lagrangian of Lin [12] and Seliger and Whitham [11], a viscous part, ℓ_{visc}, with shear and volume viscosity η, η', and a conductive part, ℓ_{cond}, with thermal conductivity λ. Denoting the specific inner energy of the fluid by $e = e(\varrho, s)$ the temperature is given by

$$T = \frac{\partial e}{\partial s}. \tag{7}$$

The presence of the logarithm term $\ln\sqrt{\bar{\chi}/\chi}$ in ℓ_{visc} and ℓ_{cond} signifies the *discontinuous* nature of the Lagrangian.

2.1.2 | Reduced Lagrangian Considering Only Thermal Conduction

For the purpose of solely evaluating the impact of heat conduction the viscous part, ℓ_{visc}, can be ignored, playing no further role in the subsequent analysis; however, for completeness it is subsequently reintegrated into the finally suggested Lagrangian—see Equation (42). This enables the number of fields to be reduced as a favorable secondary feature: followed by considering the Euler–Lagrange equation with respect to $\vec{u}$:

$$\varrho\vec{u} - \varrho\nabla\varphi - \varrho\alpha\nabla\xi - \varrho\frac{1}{\omega_0}\mathfrak{I}(\bar{\chi}\nabla\chi) = \vec{0},$$

the velocity can be expressed in terms of the other fields in a Clebsch-type [10] form:

$$\vec{u} = \nabla\varphi + \alpha\nabla\xi + \frac{1}{\omega_0}\Im(\bar{\chi}\nabla\chi), \tag{8}$$

which after insertion into (4) leads to the following reduced form of ℓ_{rev}:

$$\ell_{\text{rev}} = -\varrho\left[\partial_t\varphi + \alpha\partial_t\xi + \frac{1}{\omega_0}\Im(\bar{\chi}\partial_t\chi)\right. \\ \left.+\frac{1}{2}\left(\nabla\varphi + \alpha\nabla\xi + \frac{1}{\omega_0}\Im[\bar{\chi}\nabla\chi]\right)^2 + e\right]. \tag{9}$$

2.2 | Thermodynamic State Equations, Euler–Lagrange Equations, and Decomposition

The following state equation for the specific inner energy is considered:

$$e = c_0T_0\left[1+\frac{1}{\beta}\ln\left(\frac{\varrho}{\varrho_0}\right)\right]\exp\left(\frac{s}{c_0}\right) + e_2(\varrho) \\ = \bar{\chi}\chi + \frac{\bar{\chi}\chi}{\beta}\ln\left(\frac{\varrho}{\varrho_0}\right) + e_2(\varrho) \tag{10}$$

consisting of a purely thermal part, $\bar{\chi}\chi$, followed by a thermomechanical contribution with coupling parameter, β, and finally a purely hydroelastic part, $e_2(\varrho)$.

The Euler–Lagrange equations resulting from the Lagrangian (3) with the above state equation and in the absence ℓ_{visc} are computed in Appendix A.3, and consist of a continuity equation, a generalized Bernoulli's equation, an evolution equation for the thermal excitation, and two transport equations for the Clebsch variables.

As a consequence of (10), the relationship

$$\chi\frac{\partial e}{\partial\chi} = \bar{\chi}\chi + \frac{\bar{\chi}\chi}{\beta}\ln\left(\frac{\varrho}{\varrho_0}\right)$$

holds, allowing (6) to be rewritten as

$$\ell_{\text{cond}} = -\frac{\lambda}{i\omega_0c_0}\nabla\left(\bar{\chi}\chi\left[1+\frac{1}{\beta}\ln\left(\frac{\varrho}{\varrho_0}\right)\right]\right)\cdot\nabla\left(\frac{\ln\sqrt{\bar{\chi}/\chi}}{1+\beta^{-1}\ln(\varrho/\varrho_0)}\right), \\ = \underbrace{\frac{\lambda}{c_0\omega_0}\Im\left[\frac{\bar{\chi}}{\chi}(\nabla\chi)^2\right]}_{\ell_{\text{th}}} + \underbrace{\frac{\lambda}{c_0\omega_0}\Im(\bar{\chi}\nabla\chi)\cdot\nabla\ln\left(1+\frac{1}{\beta}\ln\left(\frac{\varrho}{\varrho_0}\right)\right)}_{\ell_{\text{th-mech}}} \\ + \underbrace{\frac{\lambda\bar{\chi}\chi}{i\omega_0c_0}\ln\sqrt{\frac{\bar{\chi}}{\chi}}\nabla\ln\left(\left[1+\frac{1}{\beta}\ln\left(\frac{\varrho}{\varrho_0}\right)\right]\frac{\bar{\chi}\chi}{c_0T_0}\right)\cdot\nabla\ln\left(1+\frac{1}{\beta}\ln\left(\frac{\varrho}{\varrho_0}\right)\right)}_{\ell_{\text{discont}}} \tag{11}$$

consisting of three contributions: (i) a purely thermal one ℓ_{th}, (ii) a continuous thermomechanical one $\ell_{\text{th-mech}}$, and (iii) a discontinuous one ℓ_{discont}.

In an earlier paper, Scholle et al. [23] suggested $\ell_{\text{cond}} \approx \ell_{\text{th}}$ as a simple approximation for the conductive part of the Lagrangian; however, this was not followed up with any analysis to prove his hypothesis since the focus of the paper was the influence of the viscosity on acoustic waves. It is therefore the aim of the present work to subject this unproven hypothesis to a critical examination and, in the case of a negative finding, to work out an alternative proposal for an approximation to the conductive term in the Lagrangian by exploring the influence of heat conduction on acoustic waves. For this purpose and to aid the reader, as in (11), different terms in subsequent equations are highlighted in color in order to better understand their individual effects on the results of the wave analysis performed.

The outcome of this investigation is by no means restricted to acoustic wave propagation. On the contrary, it is a valuable undertaking as to the suitability of an approximated Lagrangian for the modeling of compressible flow problems in general.

3 | Linear Wave Analysis

3.1 | Brief Description of the Method

In a recent article [24], a method is outlined allowing for a linear and weakly nonlinear wave analysis stemming directly from a Lagrangian: if ψ_i, $i = 1, \ldots, N$ are the fundamental fields entering the Lagrangian $\ell = \ell(\psi_i, \partial_\alpha\psi_i)$, for a given *reference state* ψ_{0i} a perturbed state:

$$\psi_i = \psi_{0i} + \tilde{\psi}_i$$

is considered where $\tilde{\psi}_i$ represents the small perturbation involved. With the objective of undertaking a linear stability analysis, a Taylor expansion of the Lagrangian with respect to $\tilde{\psi}_i$ up to quadratic order is performed, leading to a *perturbation Lagrangian* of the form

$$\Omega := \frac{1}{2}\left.\frac{\partial^2\ell}{\partial\psi_i\partial\psi_j}\right|_0\tilde{\psi}_i\tilde{\psi}_j + \left.\frac{\partial^2\ell}{\partial(\partial_\alpha\psi_i)\partial\psi_j}\right|_0(\partial_\alpha\tilde{\psi}_i)\tilde{\psi}_j \\ + \frac{1}{2}\left.\frac{\partial^2\ell}{\partial(\partial_\alpha\psi_i)\partial(\partial_\beta\psi_j)}\right|_0(\partial_\alpha\tilde{\psi}_i)(\partial_\beta\tilde{\psi}_j); \tag{12}$$

a collection of all the quadratic contributions from the Taylor expansion. By variation with respect to $\tilde{\psi}_i$, the *Jacobi equations* [4, 25, 26] result:

$$\frac{\partial\Omega}{\partial\tilde{\psi}_i} - \partial_\alpha\left(\frac{\partial\Omega}{\partial(\partial_\alpha\tilde{\psi}_i)}\right) = 0 \tag{13}$$

as the evolution equations for the perturbations. These are in fact the Euler–Lagrange equations of the perturbation Lagrangian Ω and automatically linear due to Ω being quadratic. After prudent manipulation with the aim of reducing the number of equations and to establish an equation with the character of a wave equation while neglecting nonclassical terms of order ω_0^{-2} (after time/ensemble averaging), solutions in the form of harmonic waves are assumed, implying a homogenous linear equation set (LES), the determinant of which has to vanish for nontrivial solutions, leading finally to an implicit form of dispersion relation.

3.2 | Application to the Lagrangian

3.2.1 | Associated Perturbation Lagrangian

By taking the rest state, $\varrho = \varrho_0$, $\varphi = \alpha = \xi = 0$, and $\chi = \chi_0(t) = \sqrt{c_0 T_0}\exp(-\mathrm{i}\omega_0 t)$ as a reference state and making the following substitutions:

$$\zeta := \frac{\bar{\chi}_0\tilde{\chi}}{c_0 T_0} = \frac{\tilde{\chi}}{\chi_0}, \tag{14}$$

$$\Phi := \varphi + \frac{c_0 T_0}{\omega_0}\mathfrak{I}\zeta, \tag{15}$$

the resulting perturbation Lagrangian is

$$\Omega = \overbrace{-\tilde{\varrho}\partial_t\Phi - \varrho_0\alpha\partial_t\xi - \frac{\varrho_0 c_0 T_0}{\omega_0}\mathfrak{I}\left(\bar{\zeta}\partial_t\zeta\right) - \frac{\varrho_0}{2}(\nabla\Phi)^2 - \frac{a_0^2}{2\varrho_0}\tilde{\varrho}^2 - \frac{2c_0T_0}{\beta}\tilde{\varrho}\mathfrak{R}\zeta}^{\Omega_{\mathrm{rev}}} + \underbrace{\frac{\lambda T_0}{\omega_0}\mathfrak{I}(\nabla\zeta)^2}_{\Omega_{\mathrm{th}}} + \underbrace{\frac{\lambda T_0}{\omega_0}\nabla\mathfrak{I}\zeta\cdot\frac{\nabla\tilde{\varrho}}{\beta\varrho_0}}_{\Omega_{\text{th-mech}}} + \underbrace{\frac{\lambda T_0}{\mathrm{i}\omega_0}\ln\sqrt{\frac{\bar{\chi}_0}{\chi_0}}\left[2\nabla\mathfrak{R}\zeta + \frac{\nabla\tilde{\varrho}}{\beta\varrho_0}\right]\cdot\frac{\nabla\tilde{\varrho}}{\beta\varrho_0}}_{\Omega_{\mathrm{discont}}}, \tag{16}$$

consisting of four constituent parts in accordance with the associated Lagrangian ℓ. $a_0^2 = 2\varrho_0 e_2'(\varrho_0) + \varrho_0^2 e_2''(\varrho_0)$ denotes the square of the signal speed for the reversible case (the absence of viscosity and thermal conduction).

3.2.2 | Dimensional Analysis

Dimensionless groupings allow the order of magnitude of the individual terms in equations to be estimated for many problems. It therefore makes sense to utilize this method for the Lagrangian (16) in order to estimate the three contributions to the heat conduction term, Ω_{th}, $\Omega_{\text{th-mech}}$, and $\Omega_{\mathrm{discont}}$ in relation to each other, as shown in Appendix A.4. As it turns out, since all three contributions have the same prefactor, this consideration does not lead to any findings of significance.

3.2.3 | Jacobi Equations

The Jacobi equations (13) resulting from the perturbation Lagrangian (16) are

$$\delta\tilde{\Phi}\,:\,0 = \partial_t\tilde{\varrho} + \varrho_0\nabla^2\Phi, \tag{17}$$

$$\delta\tilde{\varrho}\,:\,0 = -\partial_t\Phi - a_0^2\frac{\tilde{\varrho}}{\varrho_0} - 2\frac{c_0T_0}{\beta}\mathfrak{R}\zeta - \frac{\lambda T_0}{\varrho_0\omega_0\beta}\nabla^2\mathfrak{I}\zeta - \frac{2\lambda T_0}{\mathrm{i}\omega_0\varrho_0\beta}\ln\sqrt{\frac{\bar{\chi}_0}{\chi_0}}\nabla^2\left[\mathfrak{R}\zeta + \frac{\tilde{\varrho}}{\beta\varrho_0}\right], \tag{18}$$

$$\delta\bar{\zeta}\,:\,0 = -\frac{\varrho_0c_0T_0}{\mathrm{i}\omega_0}\partial_t\zeta - \frac{c_0T_0}{\beta}\tilde{\varrho} + \frac{\lambda T_0}{\mathrm{i}\omega_0}\nabla^2\bar{\zeta} + \frac{\lambda T_0}{2\mathrm{i}\omega_0}\frac{\nabla^2\tilde{\varrho}}{\varrho_0\beta} - \frac{\lambda T_0}{\mathrm{i}\omega_0}\ln\sqrt{\frac{\bar{\chi}_0}{\chi_0}}\frac{\nabla^2\tilde{\varrho}}{\beta\varrho_0}, \tag{19}$$

$$\delta\zeta\,:\,0 = +\frac{\varrho_0c_0T_0}{\mathrm{i}\omega_0}\partial_t\bar{\zeta} - \frac{c_0T_0}{\beta}\tilde{\varrho} - \frac{\lambda T_0}{\mathrm{i}\omega_0}\nabla^2\zeta - \frac{\lambda T_0}{2\mathrm{i}\omega_0}\frac{\nabla^2\tilde{\varrho}}{\varrho_0\beta} - \frac{\lambda T_0}{\mathrm{i}\omega_0}\ln\sqrt{\frac{\bar{\chi}_0}{\chi_0}}\frac{\nabla^2\tilde{\varrho}}{\beta\varrho_0}, \tag{20}$$

$$\delta\tilde{\alpha}\,:\,0 = -\varrho_0\partial_t\xi, \tag{21}$$

$$\delta\tilde{\xi}\,:\,0 = \varrho_0\partial_t\alpha. \tag{22}$$

From the last two equations, it follows that no vorticity is generated based on the linear approximation. Thus, the Clebsch variables α and ξ can be considered to be zero. Taking the time derivative of (18) and substituting $-\partial_t\tilde{\varrho}/\varrho_0 = \nabla^2\Phi$ according to (17), the following extended wave equation results:

$$
\begin{aligned}
&-\partial_t^2\Phi + a_0^2\nabla^2\Phi - 2\frac{c_0T_0}{\beta}\partial_t\Re\zeta \\
&\quad -\frac{\lambda T_0}{\varrho_0\omega_0\beta}\nabla^2\partial_t\Im\zeta \\
&\quad -\frac{2\lambda T_0}{\varrho_0\beta}\left[\nabla^2\Re\zeta + \frac{\nabla^2\tilde{\varrho}}{\beta\varrho_0}\right] - \frac{2\lambda T_0}{\mathrm{i}\omega_0\varrho_0\beta}\ln\sqrt{\frac{\bar{\chi}_0}{\chi_0}}\left[\nabla^2\partial_t\Re\zeta - \frac{1}{\beta}\nabla^2\left(\nabla^2\Phi\right)\right] = 0.
\end{aligned}
$$

By averaging (time or ensemble), the rapidly fluctuating terms containing $\ln\sqrt{\bar{\chi}_0/\chi_0}$ are reduced to contributions of order $\mathcal{O}\left(\omega_0^{-2}\right)$, which are due to a thermodynamic nonequilibrium [22, 23]. These are neglected subsequently. It is also expedient to decompose (19) into real and imaginary part in order to achieve separate evolution equations for $\zeta' := \Re\zeta$ and $\zeta'' := \Im\zeta$. In this way, the remaining set of equations are

$$
\partial_t\tilde{\varrho} + \varrho_0\nabla^2\Phi = 0, \tag{23}
$$

$$
\begin{aligned}
&-\partial_t^2\Phi + a_0^2\nabla^2\Phi - 2\frac{c_0T_0}{\beta}\partial_t\zeta' \\
&\quad -\frac{\lambda T_0}{\varrho_0\omega_0\beta}\nabla^2\partial_t\zeta'' - \frac{2\lambda T_0}{\varrho_0\beta}\nabla^2\left[\zeta' + \frac{\tilde{\varrho}}{\beta\varrho_0}\right] \\
&= 0,
\end{aligned} \tag{24}
$$

$$
-\partial_t\zeta' + \frac{\lambda}{\varrho_0c_0}\nabla^2\zeta' + \frac{\lambda}{2\varrho_0c_0}\frac{\nabla^2\tilde{\varrho}}{\varrho_0\beta} = 0, \tag{25}
$$

$$
\partial_t\zeta'' + \frac{\lambda}{\varrho_0c_0}\nabla^2\zeta'' + \frac{\omega_0\tilde{\varrho}}{\varrho_0\beta} = 0. \tag{26}
$$

3.2.4 | Harmonic Wave Analysis

Solutions in the form of planar harmonic waves are achieved by substituting

$$
\Phi \longrightarrow \hat{\Phi}\exp\left(\mathrm{i}\left[\vec{k}\cdot\vec{x} - \omega t\right]\right), \quad \tilde{\varrho} \longrightarrow \hat{\varrho}\exp\left(\mathrm{i}\left[\vec{k}\cdot\vec{x} - \omega t\right]\right),
$$

$$
\zeta' \longrightarrow \hat{\zeta}'\exp\left(\mathrm{i}\left[\vec{k}\cdot\vec{x} - \omega t\right]\right), \quad \zeta'' \longrightarrow \hat{\zeta}''\exp\left(\mathrm{i}\left[\vec{k}\cdot\vec{x} - \omega t\right]\right)
$$

into Equations (23–26) and multiplying each by $\exp\left(-\mathrm{i}\left[\vec{k}\cdot\vec{x} - \omega t\right]\right)$. The outcome is a homogeneous LES for the four complex amplitudes $\hat{\Phi}, \hat{\varrho}, \hat{\zeta}', \hat{\zeta}''$. On introducing the nondimensional groupings

$$
Z := \frac{\lambda k^2}{\varrho_0c_0\omega}, \qquad \tilde{\omega} := \frac{\lambda\omega}{\varrho_0c_0^2T_0}, \qquad W := \frac{a_0^2}{c_0T_0}, \qquad \varepsilon := \frac{\omega}{\omega_0}, \tag{27}
$$

the resulting LES can be written in matrix form as

$$
\begin{pmatrix}
-Z/\Omega & -\mathrm{i} & 0 & 0 \\
\beta\left(1 - \frac{WZ}{\Omega}\right) & \frac{2Z}{\beta} & 2(\mathrm{i} + Z) & -\mathrm{i}\varepsilon Z \\
0 & -\frac{Z}{2\beta} & \mathrm{i} - Z & 0 \\
0 & \frac{1}{\varepsilon\beta} & 0 & -\mathrm{i} - Z
\end{pmatrix}
\begin{pmatrix}
\omega\hat{\Phi}/(c_0T_0) \\ \hat{\varrho}/\varrho_0 \\ \hat{\zeta}' \\ \hat{\zeta}''
\end{pmatrix}
=
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{28}
$$

For nontrivial solutions, the determinant of the matrix in (28) has to vanish; leading, after multiplication by $\beta\tilde{\omega}$, to a dispersion relationship in its most general implicit form

$$
\left(1 + Z^2\right)\left[\mathrm{i}\left(\beta^2\tilde{\omega} - \beta^2WZ\right) - 2Z^2\right] + 2\mathrm{i}Z^3 + Z^3(\mathrm{i} + Z) = 0. \tag{29}
$$

If all terms are considered, the dispersion relation (29) is a quartic equation with respect to Z. However, on neglecting either the continuous thermomechanical coupling terms (highlighted red) or the discontinuous ones (highlighted blue), or both, it reduces to an equation of lower order, as shown subsequently.

Remarkably, ε does not appear in (29), while β occurs in combinations with $\tilde{\omega}$ and Z only, such that only three nondimensional products enter (29), namely, $\beta^2\tilde{\omega}$, Z, and β^2W. Consequently, the solutions of (29) can be written as

$$
Z = Z_i\left(\beta^2\tilde{\omega}; \beta^2W\right).
$$

While $\beta^2\tilde{\omega}$ and Z are dimensionless representatives of the angular frequency and the wavenumber, respectively, the combination

$$
\beta^2W = \frac{\beta^2a_0^2}{c_0T_0} \tag{30}
$$

turns out to be the only dimensionless parameter in the problem. In the case of the fluid being an ideal gas, it is shown in Appendix A.2 that it depends solely on the adiabatic exponent.

4 | Results and Discussion

4.1 | Explicit Dispersion Relations for Four Models

With reference to Equation (11), four different combinations of the contributions ℓ_{th}, $\ell_{\text{th-mech}}$, and ℓ_{discont} are considered for modeling thermal conduction, ℓ_{cond}, as follows: (i) a minimalistic model (MM) $\ell_{\text{cond}} = \ell_{\text{th}}$, which includes only the thermal excitation; (ii) a model that includes all continuous terms according to $\ell_{\text{cond}} = \ell_{\text{th}} + \ell_{\text{th-mech}}$; (iii) a reduced discontinuous model (RDM) $\ell_{\text{cond}} = \ell_{\text{th}} + \ell_{\text{discont}}$; and (iv) the consideration of all contributions according to $\ell_{\text{cond}} = \ell_{\text{th}} + \ell_{\text{th-mech}} + \ell_{\text{discont}}$. The implicit form of the dispersion relation for the latter case is already given by (29), those for the remaining three model scenarios result from omitting the associated red and/or blue highlighted terms.

In each case, either a cubic or a quartic equation must be solved to obtain the explicit form of the dispersion relation requiring identification, from among 3 or 4, of the solution that tends toward the linear dispersion relationship, $k = \omega/a_0$, in the low-frequency limit.

4.1.1 | MM

The simplest model scenario, proposed by Scholle [23], is based on neglecting both continuous and discontinuous thermomechanical coupling terms, with only the purely thermal conduction term ℓ_{th} remaining. In which case, the dispersion relation (29) reduces to

$$(1 + Z^2)(\tilde{\omega} - WZ) = 0$$

having solutions $Z_{1,2} = \pm\mathrm{i}$ and $Z_3 = \tilde{\omega}/W$. The latter implies, after making use of the groupings in (27), perfect linear dispersion, $k = \omega/a_0$, and therefore wave motion without attenuation. This means that despite the occurrence of thermal conduction as an irreversible effect, this model does not take dissipation into account.

4.1.2 | Continuous Model (CM)

If the discontinuous contribution to the Lagrangian, ℓ_{discont}, is omitted, the general dispersion relation (29) takes the form of a cubic equation

$$\beta^2(1 + Z^2)(\tilde{\omega} - WZ) + 2Z^3 = 0 \tag{31}$$

having at least one real-valued solution, which can be conveniently represented by its inverse function $\tilde{\omega} = \tilde{\omega}(Z)$ as follows:

$$\beta^2\tilde{\omega} = \left(\beta^2 W - \frac{2Z^2}{1 + Z^2}\right)Z. \tag{32}$$

The sign of Z is decisive as to whether the wave number k resulting from its root via (27) is purely real-valued or purely imaginary. For this reason, in Appendix A.2 it is proven that $\beta^2 W = \gamma/(\gamma - 1)$ for an ideal gas with adiabatic exponent γ, leading for a diatomic ideal gas to $\beta^2 W = 7/2$ and to always a positive value for the bracketed expression in the above, and therefore to positive Z and k, excluding attenuation per se. In the case of media other than ideal gases, which theoretically can have adiabatic exponents greater than 2, the sign of the bracketed expression can change, enabling wave attenuation for large wave numbers, but waves with smaller wave numbers remain undamped. Thus, it can be concluded that wave propagation without dissipation occurs within the continuous modeling approach, refuting the optimistic assessment in Scholle's [23] earlier paper.

Although in contrast to the MM above, dispersion is recognizable, the CM model allows for undamped waves as an unphysical feature as does the MM model.

Two further solutions of the cubic equation (31) exist but are not investigated here. Nevertheless, the solution (32) proves to be the one leading to linear dispersion in the low-frequency limit.

4.1.3 | RDM

Complementary to the above analysis, the discontinuous contribution to the Lagrangian, ℓ_{discont}, is now taken into account, with the continuous thermomechanical contribution $\ell_{\text{th-mech}}$ omitted. In which case, the dispersion relation (29) reduces to

$$(1 + Z^2)\left[\mathrm{i}\beta^2(\tilde{\omega} - WZ) - 2Z^2\right] = 0\,;$$

a quartic equation. As in the case of the MM, the factor $1 + Z^2$ associated with the two nonwave solutions $Z_{1,2} = \pm\mathrm{i}$ can be dropped. For the quadratic equation,

$$Z^2 + \frac{\mathrm{i}\beta^2 W}{2}Z - \frac{\mathrm{i}\beta^2\tilde{\omega}}{2} = 0, \tag{33}$$

that remains, the two solutions are

$$Z_{1,2} = \frac{\mathrm{i}\beta^2 W}{4}\left[\pm\sqrt{1 - \frac{8\mathrm{i}\tilde{\omega}}{\beta^2 W^2}} - 1\right]. \tag{34}$$

As before, only the solution that leads to the case of linear dispersion in the low-frequency limit is of interest. To find out which of the above solutions fulfills this criterion, a Taylor expansion of the square root above:

$$\sqrt{1 - \frac{8\mathrm{i}\tilde{\omega}}{\beta^2 W^2}} \approx 1 - \frac{4\mathrm{i}\tilde{\omega}}{\beta^2 W^2} + \frac{8\tilde{\omega}^2}{\beta^4 W^4}$$

leads to the approximate solutions:

$$Z_1 \approx \frac{\tilde{\omega}}{W}\left(1 + \frac{2\mathrm{i}\tilde{\omega}}{\beta^2 W^2}\right), \tag{35}$$

$$Z_2 \approx \frac{\mathrm{i}\beta^2 W}{4}\left[-2 + \frac{4\mathrm{i}\tilde{\omega}}{\beta^2 W^2} - \frac{8\tilde{\omega}^2}{\beta^4 W^4}\right] \tag{36}$$

revealing that Z_1 tends to linear dispersion for low frequency as required. Back substitution, making use of (27), yields

$$k^2 \approx \frac{\omega^2}{a_0^2}\left(1 + \frac{2\mathrm{i}T_0\lambda\omega}{\beta^2\varrho_0 a_0^4}\right),$$

which, after taking the square root and applying a Taylor expansion again, the approximate solution

$$k \approx \frac{\omega}{a_0}\sqrt{1 + \frac{2\mathrm{i}T_0\lambda\omega}{\beta^2\varrho_0 a_0^4}} \approx \frac{\omega}{a_0}\left(1 + \frac{\mathrm{i}T_0\lambda\omega}{\beta^2\varrho_0 a_0^4}\right) \quad (37)$$

for the wave number k is obtained, revealing a frequency-dependent attenuation coefficient $\mathfrak{I}k > 0$, as is to be expected classically [27, 28]. Therefore, dissipation occurs confirming that the occurrence of a discontinuous contribution to the Lagrangian is inevitable for this to be the case.

4.1.4 | All-Terms Model (ATM)

When considering all contributions in the Lagrangian, the following quartic equation:

$$Z^4 + \mathrm{i}(\beta^2 W - 3)Z^3 + (2 - \mathrm{i}\beta^2\tilde{\omega})Z^2 + \mathrm{i}\beta^2 W Z - \mathrm{i}\beta^2\tilde{\omega} = 0$$

results which, on substituting $Z = \mathrm{i}x$, takes the more convenient form:

$$x^4 + (\beta^2 W - 3)x^3 - (2 - \mathrm{i}\beta^2\tilde{\omega})x^2 - \beta^2 W x - \mathrm{i}\beta^2\tilde{\omega} = 0. \quad (38)$$

According to Cardano's Ars Magna [29], a closed-form solution of quartic equations is available; its construction is shown in detail in Appendix A.1. For the exemplary choice $\beta^2 W = 7/2$ for a diatomic ideal gas, all four solution branches prove to be complex-valued, implying nonvanishing attenuation. Also, one of the four branches tends toward a linear dispersion in the low-frequency limit. Like the RDM, the ATM correctly reflects the absorption of acoustic waves caused by heat conduction and the associated dissipation. A quantitative comparison of all four models is provided below.

4.2 | Visualization and Discussion of the Results

By defining

$$\omega_c := \frac{\varrho_0 c_0^2 T_0}{\beta^2 \lambda} \quad (39)$$

as a critical angular frequency, the nondimensional product $\beta^2\tilde{\omega}$ can be written as the dimensionless angular frequency

$$\beta^2\tilde{\omega} = \frac{\omega}{\omega_c}.$$

Alternatively, a dimensionless wavenumber results from

$$\sqrt{\beta^2 Z\tilde{\omega}} = \sqrt{\frac{\lambda k^2}{\varrho_0 c_0 \omega}\frac{\beta^2\lambda\omega}{\varrho_0 c_0^2 T_0}} = \frac{\beta\lambda k}{\varrho_0 c_0\sqrt{c_0 T_0}} = \frac{k}{k_c}, \quad (40)$$

with an associated critical wavenumber

$$k_c := \frac{\varrho_0 c_0\sqrt{c_0 T_0}}{\beta\lambda}. \quad (41)$$

Since two of the four models deliver complex-valued wave numbers, dispersion ($k' = \mathfrak{R}k$) and attenuation ($k'' = \mathfrak{I}k$) are plotted in two separate diagrams in Figure 1 against the frequency ratio, ω/ω_c, for the particular case of a diatomic ideal gas, $\beta^2 W = 7/2$.

All models, except the MM, show dispersion above the critical angular frequency, $\omega > \omega_c$. The RDM does not differ significantly from the ATM, while the CM exhibits remarkable differences.

The attenuation is predicted to be weaker for the RDM compared to the ATM, but there is very good agreement for frequencies below the critical frequency, $\omega < \omega_c$. Both the MM and the CM do not include attenuation.

The above study identifies the RDM as the most appropriate of the four models analyzed, as it is simplified compared to the ATM, but still takes into account the phenomenon of dissipation based on the subtle interaction of heat conduction with thermomechanical coupling. Overall, and considering the prior work related to viscosity [22, 23],

$$\ell = \ell_{\text{rev}} + \ell_{\text{visc}} + \underbrace{\ell_{\text{th}} + \ell_{\text{discont}}}_{\ell_{\text{cond}}} \quad (42)$$

can therefore be regarded favorably as a suitable Lagrangian for compressible viscous flows with both viscosity and thermal conduction effects accounted for.

5 | Conclusions

Of the four different model scenarios explored for the consideration of heat conduction in compressible flows by means of a variational formulation, the two simplest variants are proved not to exhibit dissipation, since they produce solutions that are undamped acoustic waves; the other two model variants, both including a discontinuous term ℓ_{discont} in the Lagrangian, correctly reproduce the phenomenon of wave attenuation, in accordance with classical theory, as a function of the square of the frequency in the low-frequency limit and thus include dissipation. This provides further evidence that dissipation in the framework of the Lagrangian formalism can be taken into account by a *strict*[2] variational principle, thus complementing earlier work [17, 21, 22] which has already shown this in the case of viscosity.

In view of the fact that the RDM, for frequencies below a critical frequency, provides an almost identical dispersion and absorption as the ATM, the continuous thermomechanical coupling term $\ell_{\text{th-mech}}$ seems to be generally dispensable. However, each of the four model variants with different levels of complexity can be justified, dependent on which physical effects need to be taken into account and which can be neglected when solving problems of interest.

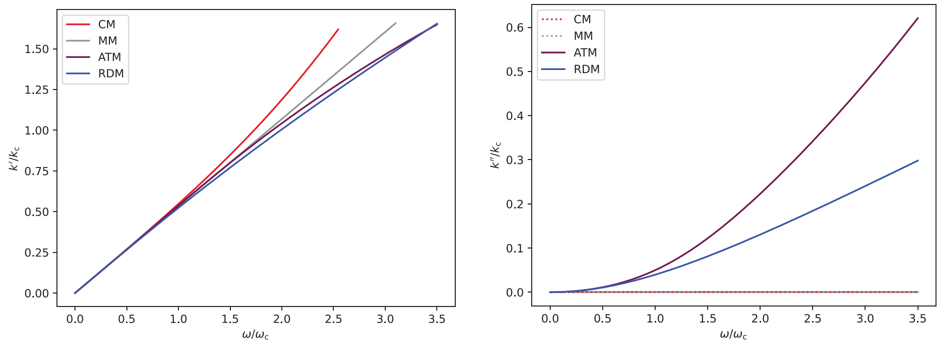

FIGURE 1 | Plots of dispersion and attenuation for the four different model scenarios, with $\beta^2 W = 7/2$ (diatomic ideal gas).

Looking ahead, it would prove worthwhile to augment the present study with a weakly nonlinear analysis via a Taylor expansion of the Lagrangian up to cubic terms, leading by variation to quadratic equations for the perturbations [24, 30], and to compare it with existing work [31, 32], where the currently neglected non-classical terms of order ω_0^{-2} are also of interest.

The primary objective and outcome of the present study is not limited to sound waves alone; rather, their analysis serves the purpose of identifying the best possible Lagrangian for compressible viscous flows with heat conduction among various alternatives. This could form the basis for the development of new solution methods, both semianalytical methods using the Ritz method and numerical methods based on finite element techniques.

Author Contributions

Markus Scholle: conceptualization, methodology, formal analysis, investigation, writing—original draft preparation, writing—review and editing, supervision, revision. **S. Ismail-Sutton**: validation, formal analysis, writing—review and editing. **Philip Gaskell**: investigation, writing—review and editing, analysis of the results, validation, supervision, revision. All authors have read and agreed to the published version of the manuscript.

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Disclosure

The authors have nothing to report.

Conflicts of Interest Statement

The authors declare no conflicts of interest.

Data Availability Statement

Data sharing not applicable to this article as no data sets were generated or analyzed during the current study.

Endnotes

[1] Total energy in the sense of kinetic energy plus inner energy including thermal contributions.

[2] In this context, "strict" means that no additional external forces are added after the variation, as frequently communicated even in recent textbooks.

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Appendix A: Calculations

A.1 | Solution of the Quartic Equation

First, the dispersion relation (38) can be written in the form

$$x^4 + Bx^3 + Cx^2 - (B+3)x - C - 2 = 0, \tag{A1}$$

with coefficients

$$B = \beta^2 W - 3,$$

$$C = -2 + \mathrm{i}\beta^2\tilde{\omega}.$$

Following the classical algorithm for finding roots of a quartic equation [29], the following auxiliary quantities are introduced:

$$a = C - \frac{3}{8}B^2, \qquad b = \frac{B^3}{8} - \frac{BC}{2} - B - 3,$$

$$P = 2 + C - \frac{C^2}{12} - \frac{B(B+3)}{4}, \qquad Q = -\frac{a^3}{27} - \frac{aP}{3} - \frac{b^2}{8},$$

$$U = \left(-\frac{Q}{2} + \sqrt{\frac{Q^2}{4} + \frac{P^3}{27}}\right)^{1/3}, \qquad z = \frac{b}{2\sqrt{2U - \frac{2a}{3} - \frac{2P}{3U}}}.$$

Finally, the four roots of the quartic equation result as

$$x_j = \frac{1}{2}\left[s_j\sqrt{2U - \frac{2a}{3} - \frac{2P}{3U}} - (-1)^j\sqrt{\frac{2P}{3U} - \frac{4a}{3} - 2U - 4s_j z}\right] - \frac{B}{4}, \quad j \in \{1,2,3,4\} \tag{A2}$$

with $s_1 = s_2 = 1$ and $s_3 = s_4 = -1$. The above algorithm has been implemented in Python.

A.2 | Parameters β, W, and $\beta^2 W$ for an Ideal Gas

From the state equation (10), the temperature is obtained via (7) as

$$T = \frac{\partial e}{\partial s} = T_0\left[1 + \frac{1}{\beta}\ln\left(\frac{\varrho}{\varrho_0}\right)\right]\exp\left(\frac{s}{c_0}\right).$$

By taking the derivative with respect to ϱ and evaluating the expression for the equilibrium state, $s = 0, \varrho = \varrho_0$, the relationship

$$\left.\frac{\partial T}{\partial \varrho}\right|_0 = \frac{T_0}{\beta\varrho_0} \tag{A3}$$

is obtained. For an ideal gas, the state equation $p/\varrho = RT/M$ with universal gas constant R and molar mass M applies:

$$\left.\frac{\partial T}{\partial \varrho}\right|_0 = \frac{M}{R}\left.\left(\frac{1}{\varrho}\frac{\partial p}{\partial \varrho} - \frac{p}{\varrho^2}\right)\right|_0 = \frac{M}{R}\left(\frac{K_0}{\varrho_0^2} - \frac{p_0}{\varrho_0^2}\right) = \frac{M}{R}\frac{a_0^2}{\varrho_0} - \frac{T_0}{\varrho_0}, \tag{A4}$$

where $K_0 = \varrho_0 a_0^2$ is the compression modulus. Finally, the speed of sound for an ideal gas fulfills the relationship

$$a_0^2 = \gamma\frac{p_0}{\varrho_0} = \gamma\frac{R}{M}T_0, \tag{A5}$$

where γ is the adiabatic exponent. By inserting (A5) into (A4) and comparing the outcome with (A3), the thermomechanical coupling coefficient results as

$$\beta = \frac{1}{\gamma - 1}. \tag{A6}$$

Reconsidering (A5), the parameter W defined in (27) yields

$$W = \frac{a_0^2}{c_0 T_0} = \gamma\frac{RT_0}{Mc_0T_0} = \gamma\frac{R}{c_m} = \gamma(\gamma - 1), \tag{A7}$$

where $c_m = R/(\gamma - 1)$ is the molar heat capacity of the gas. Finally, the decisive parameter $\beta^2 W$ turns out to be

$$\beta^2 W = \frac{\gamma}{\gamma - 1}. \tag{A8}$$

As an example, for a diatomic gas ($\gamma = 7/5$) the parameter values turn out to be: $\beta = 5/2$, $W = 14/25$, and $\beta^2 W = 7/2$.

A.3 | Euler–Lagrange Equations

Using the abbreviation $\varkappa = 1 + \ln(\varrho/\varrho_0)/\beta$, the Euler–Lagrange equations associated to (3), with ℓ_{visc} neglected, read:

$$\delta\varphi \,:\, 0 = \partial_t \varrho + \nabla \cdot (\varrho \vec{u}), \tag{A9}$$

$$\delta\varrho \,:\, 0 = \frac{\ell_{\text{rev}}}{\varrho} - \frac{\bar{\chi}\chi}{\beta} - \varrho e_2'(\varrho) + \frac{\lambda \ln\sqrt{\bar{\chi}/\chi}}{\mathrm{i}\omega_0 c_0 \varrho \beta \varkappa^2} \nabla^2(\varkappa\bar{\chi}\chi), \tag{A10}$$

$$\delta\bar{\chi} \,:\, 0 = -\frac{\varrho}{\mathrm{i}\omega_0}\{\partial_t + \vec{u}\cdot\nabla\}\chi - \varrho\varkappa\chi + \frac{\lambda\varkappa\chi}{\mathrm{i}\omega_0 c_0}\left[\nabla^2\left(\frac{\ln\sqrt{\bar{\chi}/\chi}}{\varkappa}\right) + \frac{\nabla^2(\varkappa\bar{\chi}\chi)}{2\varkappa^2\bar{\chi}\chi}\right], \tag{A11}$$

$$\delta\alpha \,:\, 0 = -\varrho\{\partial_t + \vec{u}\cdot\nabla\}\xi, \tag{A12}$$

$$\delta\xi \,:\, 0 = \partial_t(\varrho\alpha) + \nabla\cdot(\varrho\alpha\vec{u}), \tag{A13}$$

where the state equation (10) has been considered, and consist of the continuity equation (A9), a generalized Bernoulli's equation (A10) [10, 33], an evolution equation (A11) for the thermal excitation (variation with respect to χ delivers its complex conjugate) considering both convection and conduction, and transport equations (A12), (A13) for the Clebsch variables, the latter being related to the vortex dynamics and conservation of circulation [8–10, 33].

A.4 | Dimensionless Form of the Perturbation Lagrangian

By introducing the dimensionless fields

$$\varrho^* := \frac{\tilde{\varrho}}{\varrho_0}, \qquad \Phi^* = \frac{\omega\Phi}{c_0 T_0}, \qquad \xi^* = \frac{\omega\xi}{c_0 T_0}, \tag{A14}$$

and the dimensionless differential operators

$$\partial_t^* = \frac{1}{\omega}\partial_t, \qquad \nabla^* := k^{-1}\nabla, \tag{A15}$$

the perturbation Lagrangian (16) can be written in the following dimensionless form:

$$\frac{\Omega}{\varrho_0 c_0 T_0} = -\varrho^*\partial_t^*\Phi^* - \alpha\partial_t^*\xi^* - \varepsilon\mathfrak{I}\left(\bar{\zeta}\partial_t^*\zeta\right) - \frac{Z}{2\tilde{\omega}}\left(\nabla^*\Phi^*\right)^2 - \frac{W}{2}\varrho^{*2} - \frac{2\varrho^*}{\beta}\mathfrak{R}\zeta + \varepsilon Z\left[\mathfrak{I}\left(\nabla^*\zeta\right)^2 + \frac{1}{\beta}\nabla^*\mathfrak{I}\zeta\cdot\nabla^*\varrho^* - \frac{\mathrm{i}}{\beta}\ln\sqrt{\frac{\bar{\chi}_0}{\chi_0}}\left(2\nabla^*\mathfrak{R}\zeta + \frac{1}{\beta}\nabla^*\varrho^*\right)\cdot\nabla^*\varrho^*\right] \tag{A16}$$

containing the parameters defined in (27) as nondimensional scales. Since all three contributions to heat conduction (second line) have the same scale εZ as prefactor, no decision can be made on the basis of the above dimensional analysis as to which contribution(s) might be negligible compared to the others.