

## GRADIENT-DEPENDENT TRANSPORT COEFFICIENTS IN THE NAVIER–STOKES–FOURIER SYSTEM

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**ABSTRACT.** In the engineering praxis, Newton’s law of viscosity and Fourier’s heat conduction law are applied to describe thermomechanical processes of fluids. Despite several successful applications, there are some obscure and unexplored details, which are partly answered in this paper using the methodology of irreversible thermodynamics. Liu’s procedure is applied to derive the entropy production rate density, in which positive definiteness is ensured via linear Onsagerian equations; these equations are exactly Newton’s law of viscosity and Fourier’s heat conduction law. The calculations point out that, theoretically, the transport coefficients (thermal conductivity and viscosity) can also depend on the gradient of the state variables in addition to the well-known dependence of the state variables. This gradient dependency of the transport coefficients can have a significant impact on the modeling of such phenomena as welding, piston effect or shock waves.

### 1. Introduction

In engineering practice, classical constitutive laws such as Newton’s law of viscosity and Fourier’s heat conduction law are still fundamental and have been used successfully in several situations. These constitutive laws, together with the balance equations, form the Navier–Stokes–Fourier system. However, as with any other models in physics, these also have a limited range of validity. There are situations and phenomena which could outreach that limit, and thus, a reliable and practically helpful explanation is necessary by revisiting the background of these models.

In irreversible thermodynamics, various approaches exist, and they provide numerous ideas about the generalization possibilities. For instance, the Rational Extended Thermodynamics [1] approach considers compatibility with kinetic theory rigorously. Hence, it best works for rarefied gas systems and is much less advantageous for room temperature solids. The Extended Irreversible Thermodynamic [2] approach treats kinetic theory loosely, leaving open the possibilities for adapting

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any suitable elements. Furthermore, that approach utilizes only dissipative fluxes as extra state variables, therefore limiting the possibilities when other types of state variables would be necessary (e.g. the fabric density in fracture mechanics [3]). Internal Variable Methodology [4] extends the possibilities by allowing other variables beyond dissipative fluxes and also treats the entropy flux more flexibly [5–7].

Although the classical continuum thermodynamic background for the Navier–Stokes–Fourier system is known (see e.g. [8,9]) and its several extensions and generalizations are already existing, its review with the tools of modern irreversible thermodynamics helps improve the understanding and provide ideas about their extensions and possible couplings.

This is exactly our aim in the present paper: starting with the balance equations and the dissipation inequality, the transport equations for the classical Navier–Stokes–Fourier system is derived via Liu’s procedure [10]. Liu’s procedure, a rigorous mathematical technique provides further insight into both classical and generalized theories. Furthermore, it also reveals the possible—and non-trivial—nonlinearities (state variable dependency). The main result of this investigation is that transport coefficients can depend not only on the state variables, but their gradients, too. This kind of dependence can have a great impact on the modeling of such phenomena, in which sudden changes appear, such as welding [11], piston effect [12] or shock waves [13].

## 2. The Navier–Stokes–Fourier system

In general, continuum theories are formed by balance equations and constitutive equations (also including thermostatic relationships and transport equations). While balance equations express the conservation of extensive quantities independent of the material and hence describe dynamics, constitutive equations characterize the material itself. More closely, thermostatic relationships connect the extensive and intensive state variables through the entropy function, and, in parallel, transport equations assemble relationships among the thermodynamical fluxes and forces. These latter ones are usually the gradients of intensive state variables.

**2.1. Balance equations.** Let us assume a one-component non-polar fluid, and only the thermomechanical interactions are considered. Neglecting volumetric source terms such as field strength or heat sources, the substantial forms of the conservation of mass, linear momentum, and total energy are

$$(2.1) \quad \dot{\rho} + \rho \nabla \cdot \mathbf{v} = 0,$$

$$(2.2) \quad \rho \dot{\mathbf{v}} + \mathbf{P} \cdot \nabla = \mathbf{0},$$

$$(2.3) \quad \rho \dot{e} + \nabla \cdot \mathbf{J}_E = 0,$$

where  $\rho$ ,  $\mathbf{v}$  and  $e$  are the density, velocity field and (mass) specific total energy, respectively,  $\mathbf{P} = \mathbf{P}^T$  is the symmetric pressure tensor (here  $^T$  denotes the transpose of a second order tensor), which is a consequence of the conservation of angular momentum,  $\mathbf{J}_E$  is the current density of total energy. The substantial or comoving

$$\dot{\bullet} := \partial_t \bullet + (\bullet \otimes \nabla) \cdot \mathbf{v}$$

characterizes the change of a quantity in time at a fixed material point, while it flows with velocity  $\mathbf{v}$ , here and later on  $\partial_t$  denotes the partial time derivative, and  $\nabla$  is the nabla operator, which represents gradient or divergence depending on the tensorial multiplication.

**2.2. Constitutive equations.** The second law of thermodynamics, i.e. the thermodynamical stability of

- the material itself,
- and the realized process

is expressed through entropy. The first part belongs to thermostatic considerations, while the second one prescribes requirements on the dynamics.

2.2.1. *Thermostatic constitution.* Now, we briefly summarize the thermostatic properties of the material, which is in connection with the entropy, hence, the main properties of entropy are collected here:

- (1) There exist independent thermodynamical bodies, which are characterized by extensive state variables. The thermodynamical state space is spanned by these extensive state variables, namely, the internal energy  $U$ , the volume  $V$ , and the mass  $m$ . Entropy  $S$  is a potential function of the state space in the variables  $(U, V, m)$ , from which the intensive state functions, more closely temperature  $T$ , pressure  $p$ , and the chemical potential  $\mu$  follow as

$$\begin{aligned}\frac{\partial S}{\partial U}\Big|_{V,m} &= \frac{1}{T}(U, V, m), \\ \frac{\partial S}{\partial V}\Big|_{U,m} &= \frac{p}{T}(U, V, m), \\ \frac{\partial S}{\partial m}\Big|_{U,V} &= -\frac{\mu}{T}(U, V, m),\end{aligned}$$

respectively. This relationship is expressed through the Gibbs relation

$$(2.4) \quad dS = \frac{1}{T}dU + \frac{p}{T}dV - \frac{\mu}{T}dm.$$

- (2) Entropy is an extensive state function.
  - (a) More precisely, entropy is a first-order Euler homogeneous function of its variables. For example

$$(2.5) \quad S(c \cdot U, c \cdot V, c \cdot m) = c \cdot S(U, V, m)$$

with the positive constant  $c$ .

- (b) From the previous statement, the introduction of specific entropy follows. The mass-specific entropy (later called specific entropy) is defined as

$$(2.6) \quad s(u, v) := \frac{1}{m}S\left(\frac{U}{m}, \frac{V}{m}\right)$$

with  $u = \frac{U}{m}$  and  $v = \frac{V}{m}$  denoting the (mass) specific internal energy and specific volume, respectively. Analogously, the volume-specific

entropy, also known as the entropy density, is

$$(2.7) \quad \varrho_S(\varrho, \varrho_U) := \frac{1}{V} S\left(\frac{U}{V}, \frac{m}{V}\right),$$

where  $\varrho_U = \frac{U}{V}$  and  $\varrho = \frac{m}{V}$  are the internal energy density and the (mass) density, respectively.

(c) The Euler relation for the entropy is

$$(2.8) \quad S(U, V, m) = \frac{1}{T}(U, V, m)U + \frac{p}{T}(U, V, m)V - \frac{\mu}{T}(U, V, m)m.$$

As consequences of (2.4), (2.5), (2.6), (2.7) and (2.8) the specific entropy and the entropy density are

$$\begin{aligned} s(u, v) &= \frac{1}{T}(u, v)u + \frac{p}{T}(u, v)v - \frac{\mu}{T}(u, v), \\ \varrho_S(\varrho_U, \varrho) &= \frac{1}{T}(\varrho_U, \varrho)\varrho_U + \frac{p}{T}(\varrho_U, \varrho) - \frac{\mu}{T}(\varrho_U, \varrho)\varrho, \end{aligned}$$

and the Gibbs relation on the specific entropy and the entropy density are

$$(2.9) \quad \begin{aligned} ds &= \frac{1}{T}du + \frac{p}{T}dv, \\ d\varrho_S &= \frac{1}{T}d\varrho_U - \frac{\mu}{T}d\varrho, \end{aligned}$$

respectively.

(3) The specific entropy is a concave function of its variables, i.e.

$$\frac{\partial^2 s}{\partial u^2} \Big|_v \geq 0, \quad \frac{\partial^2 s}{\partial v^2} \Big|_u \geq 0, \quad \det \nabla_{(u,v)} s \geq 0.$$

The so-called internal stability criteria on the isochoric specific heat capacity

$$c_v := \frac{\partial u}{\partial T} \Big|_v > 0$$

and isothermal compressibility coefficient

$$\chi_T := -\frac{1}{v} \frac{\partial v}{\partial p} \Big|_T > 0$$

follows from this condition (or vice versa), which actually realizes the Le Châtelier–Braun principle. These describe relationships among changes irrespective of what external actions have created those changes.

Next to the isochoric specific heat capacity and isothermal compressibility coefficient

- the isobaric thermal expansion coefficient  $\beta_p := \frac{1}{v} \frac{\partial v}{\partial T} \Big|_p$  and
- the isobaric specific heat capacity  $c_p := c_v - T \left( \frac{\partial p}{\partial T} \Big|_v \right)^2 / \frac{\partial p}{\partial v} \Big|_T = c_v + T v \frac{\beta_p^2}{\chi_T}$

is applied to characterize the thermostatic behavior of the material. There is no restriction on the sign of  $\beta_p$ . Usually, it is positive, however, e.g., in the case of water between 0°C and 4°C it is negative. From the conditions  $T > 0$ ,  $v > 0$

and  $\chi_T > 0$  follows that  $c_p \geq c_v$ , and equality exist when thermal expansion is neglected.

2.2.2. *Constitution on the transport properties.* The second part of the second law prescribes conditions on the dynamics, which is expressed through entropy production. The balance of entropy reads as

$$(2.10) \quad \rho \dot{s} + \nabla \cdot \mathbf{J}_S = \Sigma_S$$

with the entropy current density  $\mathbf{J}_S$  and the entropy production rate density  $\Sigma_S$ , which is a positive semi-definite function along a realized process, i.e.,  $\Sigma_S \geq 0$ , thus ensuring dynamic stability of the process. It means that positive semi-definiteness of the entropy production rate density imposes constraints on the transport properties. (2.10) is frequently given via the dissipation inequality

$$0 \leq \rho \dot{s} + \nabla \cdot \mathbf{J}_S.$$

From a mathematical point of view, the balances (2.1)–(2.3) are constraints to evaluate the dissipation inequality. Here, we apply a rigorous mathematical technique, namely Liu's procedure. Liu's procedure specifies the entropy production rate density and the relationship of entropy current density to the thermodynamical currents, too. Furthermore, it also highlights the possible state variable dependence of the transport properties.

Liu's procedure is based on Liu's theorem, which is a special case of Farkas' lemma on conditional algebraic inequalities [14, 15]. Briefly, the inequality

$$(2.11) \quad \boldsymbol{\alpha}(\hat{\mathbf{x}}) \cdot \mathbf{y} + \beta(\hat{\mathbf{x}}) \geq 0,$$

holds for all  $\mathbf{y}$  such that

$$(2.12) \quad \mathbf{A}(\hat{\mathbf{x}}) \cdot \mathbf{y} + \mathbf{B}(\hat{\mathbf{x}}) = \mathbf{0},$$

if and only if there exists  $\boldsymbol{\Lambda}$ -called Lagrange–Farkas multiplier–such that

$$(2.13) \quad \boldsymbol{\alpha}(\hat{\mathbf{x}}) - \boldsymbol{\Lambda} \cdot \mathbf{A}(\hat{\mathbf{x}}) = \mathbf{0},$$

$$(2.14) \quad \beta(\hat{\mathbf{x}}) - \boldsymbol{\Lambda} \cdot \mathbf{B}(\hat{\mathbf{x}}) \geq 0.$$

Here and later on  $\mathbf{x}$  denotes the variables, which span the *thermodynamical state space* (the basic variables),  $\hat{\mathbf{x}}$  the elements of the *constitutive state space*, which in general contains  $\mathbf{x}$  and its temporal and spatial derivatives,  $\mathbf{y}$  contains the elements of the *process direction space*, which is spanned by the derivatives of the constitutive variables  $\hat{\mathbf{x}}$  that are not already given in  $\hat{\mathbf{x}}$ . Furthermore,  $\mathbf{A}$ ,  $\mathbf{B}$ ,  $\boldsymbol{\alpha}$  and  $\beta$  contains the derivatives of the *constitutive functions* with respect to the constitutive variables. Usually, equations (2.11) and (2.12) together are called Coleman–Mizel formulation of continuum thermodynamics, equation (2.13) is called Liu-equation and (2.14) is the dissipation inequality. For deeper mathematical details, see e.g. the appendices of [16] and [17].

Usually, Liu's procedure is utilized in the local description. However, now we perform the calculations in the substantial one due to two reasons:

- First, the formulas in the substantial description are more transparent;

- Second, the substantial description is much more connected to the material itself, than the local one. Therefore, thermodynamical calculations, including Liu's procedure, are more natural in the present approach.

In order to check the results, we have realized these calculations in the local description as well, leading to the same outcome. Furthermore, [1] also presents this approach, which connects Galilean invariance to the Lagrange–Farkas multipliers, on which in this case [1] refers as internal Lagrange multipliers.

Let us present Liu's procedure applied to the Navier–Stokes–Fourier system. First, one has to fix variables and functions. The state space is spanned by the variables  $\mathbf{x} := (\varrho, \mathbf{v}, e)$ . In case of Navier–Stokes–Fourier system—as a basic example of classical irreversible thermodynamics—the constitutive state space is spanned by  $\hat{\mathbf{x}} := (\varrho, \mathbf{v}, e, \nabla\varrho, \mathbf{v} \otimes \nabla, \nabla e)$ , thus the process direction space is spanned by  $\mathbf{y} := (\dot{\varrho}, \dot{\mathbf{v}}, \dot{e}, (\nabla\dot{\varrho}), (\mathbf{v} \otimes \nabla), (\nabla\dot{e}), (\nabla\dot{\varrho}) \otimes \nabla, (\mathbf{v} \otimes \nabla) \otimes \nabla, (\nabla\dot{e}) \otimes \nabla)$ . The constitutive functions are  $(s, \mathbf{P}, \mathbf{J}_E, \mathbf{J}_S)$ .

According to Liu's procedure, the dissipation inequality constrained by the balances (2.1)–(2.3) reads as

$$\begin{aligned}
(2.15) \quad & 0 \leq \varrho \dot{s} + \nabla \cdot \mathbf{J}_S - b_1(\dot{\varrho} + \varrho \nabla \cdot \mathbf{v}) - \mathbf{b}_2 \cdot (\varrho \dot{\mathbf{v}} + \mathbf{P} \cdot \nabla) - b_3(\varrho \dot{e} + \nabla \cdot \mathbf{J}_E) \\
& = \left( \varrho \frac{\partial s}{\partial \varrho} - b_1 \right) \dot{\varrho} + \varrho \left( \frac{\partial s}{\partial \mathbf{v}} - \mathbf{b}_2 \right) \cdot \dot{\mathbf{v}} + \varrho \left( \frac{\partial s}{\partial e} - b_3 \right) \dot{e} + \varrho \frac{\partial s}{\partial (\nabla \varrho)} \cdot (\nabla \dot{\varrho}) \\
& \quad + \varrho \frac{\partial s}{\partial (\mathbf{v} \otimes \nabla)} : (\mathbf{v} \otimes \nabla) + \varrho \frac{\partial s}{\partial (\nabla e)} \cdot (\nabla \dot{e}) + \left( \frac{\partial \mathbf{J}_S}{\partial \varrho} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial \varrho} - b_3 \frac{\partial \mathbf{J}_E}{\partial \varrho} \right) \cdot \nabla \varrho \\
& \quad + \left( \frac{\partial \mathbf{J}_S}{\partial \mathbf{v}} - b_1 \varrho \mathbf{1} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial \mathbf{v}} - b_3 \frac{\partial \mathbf{J}_E}{\partial \mathbf{v}} \right) : (\mathbf{v} \otimes \nabla) \\
& \quad + \left( \frac{\partial \mathbf{J}_S}{\partial e} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial e} - b_3 \frac{\partial \mathbf{J}_E}{\partial e} \right) \cdot \nabla e \\
& \quad + \left( \frac{\partial \mathbf{J}_S}{\partial (\nabla \varrho)} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial (\nabla \varrho)} - b_3 \frac{\partial \mathbf{J}_E}{\partial (\nabla \varrho)} \right) : [(\nabla \varrho) \otimes \nabla] \\
& \quad + \left( \frac{\partial \mathbf{J}_S}{\partial (\mathbf{v} \otimes \nabla)} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial (\mathbf{v} \otimes \nabla)} - b_3 \frac{\partial \mathbf{J}_E}{\partial (\mathbf{v} \otimes \nabla)} \right) : [(\mathbf{v} \otimes \nabla) \otimes \nabla] \\
& \quad + \left( \frac{\partial \mathbf{J}_S}{\partial (\nabla e)} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial (\nabla e)} - b_3 \frac{\partial \mathbf{J}_E}{\partial (\nabla e)} \right) : [(\nabla e) \otimes \nabla].
\end{aligned}$$

The Liu equations are obtained from the previous inequality as the multipliers of the independent elements of the process direction space, i.e.,

$$\begin{aligned}
(2.16) \quad & \dot{\varrho} : & \varrho \frac{\partial s}{\partial \varrho} - b_1 &= 0, \\
& \dot{\mathbf{v}} : & \frac{\partial s}{\partial \mathbf{v}} - \mathbf{b}_2 &= \mathbf{0}, \\
& \dot{e} : & \frac{\partial s}{\partial e} - b_3 &= 0, \\
(2.17) \quad & (\nabla \dot{\varrho}) : & \varrho \frac{\partial s}{\partial (\nabla \varrho)} &= \mathbf{0},
\end{aligned}$$

$$\begin{aligned}
(2.18) \quad (\mathbf{v} \otimes \nabla): & \quad \varrho \frac{\partial s}{\partial(\mathbf{v} \otimes \nabla)} = \mathbf{0}, \\
(\nabla e): & \quad \varrho \frac{\partial s}{\partial(\nabla e)} = \mathbf{0}, \\
(2.19) \quad (\nabla \varrho) \otimes \nabla: & \quad \frac{\partial \mathbf{J}_S}{\partial(\nabla \varrho)} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial(\nabla \varrho)} - b_3 \frac{\partial \mathbf{J}_E}{\partial(\nabla \varrho)} = \mathbf{0}, \\
(2.20) \quad (\mathbf{v} \otimes \nabla) \otimes \nabla: & \quad \frac{\partial \mathbf{J}_S}{\partial(\mathbf{v} \otimes \nabla)} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial(\mathbf{v} \otimes \nabla)} - b_3 \frac{\partial \mathbf{J}_E}{\partial(\mathbf{v} \otimes \nabla)} = \not\equiv, \\
(2.21) \quad (\nabla e) \otimes \nabla: & \quad \frac{\partial \mathbf{J}_S}{\partial(\nabla e)} - \mathbf{b}_2 \cdot \frac{\partial \mathbf{P}}{\partial(\nabla e)} - b_3 \frac{\partial \mathbf{J}_E}{\partial(\nabla e)} = \mathbf{0}.
\end{aligned}$$

Equations (2.16)–(2.18) prescribe conditions on the specific entropy, according to (2.17)–(2.18) specific entropy is independent on the gradients; thus, specific entropy is a function of  $\mathbf{x}$ , i.e.  $s = s(\mathbf{x})$ , for which the Gibbs-relation is

$$(2.22) \quad ds = \frac{\partial s}{\partial \varrho} d\varrho + \frac{\partial s}{\partial \mathbf{v}} \cdot d\mathbf{v} + \frac{\partial s}{\partial e} de = \frac{b_1}{\varrho} d\varrho + \mathbf{b}_2 \cdot d\mathbf{v} + b_3 de.$$

Integrating equations (2.19)–(2.21) with respect to the gradients the entropy current density is obtained in the form of

$$(2.23) \quad \mathbf{J}_S(\hat{\mathbf{x}}) = \frac{\partial s}{\partial \mathbf{v}}(\mathbf{x}) \cdot \mathbf{P}(\hat{\mathbf{x}}) + \frac{\partial s}{\partial e}(\mathbf{x}) \mathbf{J}_E(\hat{\mathbf{x}}) + \hat{\mathbf{J}}_S(\mathbf{x}),$$

where  $\hat{\mathbf{J}}_S$  denotes a residual entropy current density, which is assumed as zero. Since the coefficients of (2.19) and (2.21), i.e.  $(\nabla \varrho)$  and  $(\nabla e)$  are symmetric tensors, and the coefficient of (2.20), i.e.  $(\mathbf{v} \otimes \nabla)$  is symmetric in its second and third indices, Liu's procedure provides information only about the dependence of symmetrical parts. A further and open question is how the antisymmetric parts of these quantities contribute to entropy current density. Since entropy production remains unchanged when these antisymmetric parts also appear, thus the physical content stay unchanged. However, this property together with the residual entropy current density may be exploitable in numerics.

Replacing our previous results in (2.15) we obtain

$$\begin{aligned}
(2.24) \quad 0 & \leq \left( \frac{\partial}{\partial \varrho} \frac{\partial s}{\partial \mathbf{v}} \cdot \mathbf{P} + \frac{\partial}{\partial \varrho} \frac{\partial s}{\partial e} \mathbf{J}_E \right) \cdot \nabla \varrho \\
& + \left( \frac{\partial}{\partial \mathbf{v}} \otimes \frac{\partial s}{\partial \mathbf{v}} \cdot \mathbf{P} - \varrho^2 \frac{\partial s}{\partial \varrho} \mathbf{1} - \frac{\partial}{\partial \mathbf{v}} \frac{\partial s}{\partial e} \otimes \mathbf{J}_E \right) : (\mathbf{v} \otimes \nabla) \\
& + \left( \frac{\partial}{\partial e} \frac{\partial s}{\partial \mathbf{v}} \cdot \mathbf{P} + \frac{\partial}{\partial e} \frac{\partial s}{\partial e} \mathbf{J}_E \right) \cdot \nabla e \\
& = \left( \frac{\partial s}{\partial \mathbf{v}} \right) \otimes \nabla : \mathbf{P} + \nabla \left( \frac{\partial s}{\partial e} \right) \cdot \mathbf{J}_E - \varrho^2 \frac{\partial s}{\partial \varrho} \mathbf{1} : (\mathbf{v} \otimes \nabla).
\end{aligned}$$

Applying the well-known relationship among the specific total energy, the specific internal energy, and the specific kinetic energy

$$(2.25) \quad e = u + \frac{1}{2} \mathbf{v} \cdot \mathbf{v}$$

the Gibbs-relation is

$$ds = \frac{1}{T} du - \frac{p}{\rho^2 T} d\rho = \frac{1}{T} de - \frac{\mathbf{v}}{T} \cdot d\mathbf{v} - \frac{p}{\rho^2 T} d\rho,$$

where we applied that  $dv = -\frac{1}{\rho^2} d\rho$  and equations (2.9) and (2.22), hence the partial derivatives of the specific entropy with respect to  $(\rho, \mathbf{v}, e)$  are

$$\frac{\partial s}{\partial e} = \frac{1}{T}, \quad \frac{\partial s}{\partial \mathbf{v}} = -\frac{\mathbf{v}}{T}, \quad \frac{\partial s}{\partial \rho} = -\frac{p}{\rho^2 T}.$$

Substituting these derivatives into (2.24) one obtains

$$(2.26) \quad 0 \leq -\left(\frac{\mathbf{v}}{T}\right) \otimes \nabla : \mathbf{P} + \nabla \left(\frac{1}{T}\right) \cdot \mathbf{J}_E + \frac{p}{T} \mathbf{1} : (\mathbf{v} \otimes \nabla) \\ = -\frac{1}{T} (\mathbf{P} - p\mathbf{1}) : (\mathbf{v} \otimes \nabla) + (\mathbf{J}_E - \mathbf{v} \cdot \mathbf{P}) \cdot \nabla \left(\frac{1}{T}\right).$$

Here, we can recognize the usual and well-known quadratic expression of thermodynamic forces and fluxes with the dissipative fluxes

$$(2.27) \quad \begin{aligned} \mathbf{\Pi}(\hat{\mathbf{x}}) &:= \mathbf{P}(\hat{\mathbf{x}}) - p(\mathbf{x})\mathbf{1}, \\ \mathbf{J}_Q(\hat{\mathbf{x}}) &:= \mathbf{J}_E(\hat{\mathbf{x}}) - \mathbf{v} \cdot \mathbf{P}(\hat{\mathbf{x}}), \end{aligned}$$

where the first one is the viscous pressure tensor and the latter one is the heat current density. Assuming isotropy—thus different tensorial orders and characters do not couple according to Curie's principle [8]—the positive semi-definiteness of (2.26) is ensured via the linear Onsagerian equations

$$(2.28) \quad \mathbf{J}_Q(\hat{\mathbf{x}}) = l(\hat{\mathbf{x}}) \cdot \nabla \left(\frac{1}{T}(\mathbf{x})\right) = -\lambda(\hat{\mathbf{x}}) \nabla(T(\mathbf{x})),$$

$$(2.29) \quad \mathbf{\Pi}(\hat{\mathbf{x}}) = -\frac{\mu^{\text{Vol}}(\hat{\mathbf{x}}) - \mu^{\text{Sh}}(\hat{\mathbf{x}})}{3} (\nabla \cdot \mathbf{v}) \mathbf{1} - \frac{\mu^{\text{Sh}}(\hat{\mathbf{x}})}{2} (\mathbf{v} \otimes \nabla + \nabla \otimes \mathbf{v}),$$

where  $\lambda = \frac{l}{T^2} \geq 0$  denotes the thermal conductivity, while  $\mu^{\text{Vol}} \geq 0$  and  $\mu^{\text{Sh}} \geq 0$  are the volumetric and shear viscosity coefficients.

Our analysis with Liu's procedure resulted in the same constitutive functions as classical irreversible thermodynamics with some notable differences. Since the state space was fixed from the beginning of the analysis, the dependence of the constitutive functions and quantities on the state space is determined. As the indicated variable dependence shows, in general, the transport coefficients in (2.28)–(2.29) can depend on the gradient variables, too.

Now, let us determine the entropy current density in the light of our results so far, thus replacing (2.27) into (2.23) the well-known relationship between the entropy current density and heat current density is obtained, i.e.

$$\mathbf{J}_S(\mathbf{y}) = -\frac{\mathbf{v}}{T}(\bar{\mathbf{y}}) \cdot \mathbf{P}(\mathbf{y}) + \frac{1}{T}(\bar{\mathbf{y}}) \mathbf{J}_E(\mathbf{y}) = \frac{1}{T}(\mathbf{J}_E - \mathbf{v} \cdot \mathbf{P}) = \frac{1}{T} \mathbf{J}_Q.$$

The relationship among the specific total energy, the specific internal energy and the specific kinetic energy (2.25) establishes a connection between the balances



of linear momentum (2.2) and total energy (2.3), i.e.

$$0 = \varrho \dot{e} + \nabla \cdot \mathbf{J}_E \stackrel{(2.25)}{=} \stackrel{(2.27)}{=} \varrho \dot{u} + \nabla \cdot \mathbf{J}_Q + \mathbf{v} \cdot (\varrho \dot{\mathbf{v}} + \nabla \cdot \mathbf{P}) + \mathbf{P} : (\mathbf{v} \otimes \nabla),$$

where the third expression is exactly the balance of linear momentum (2.2), thus the well-known balance equation of internal energy

$$\varrho \dot{u} + \nabla \cdot \mathbf{J}_Q = -\mathbf{P} : (\mathbf{v} \otimes \nabla)$$

follows.

### 3. Analysis and conclusions

In the engineering praxis, thermomechanical processes of fluids are modeled via the Navier–Stokes–Fourier system, which is formed by the balances of mass, linear momentum, and internal energy, thermostatic constitutive equations on temperature, pressure, and constitutive equations on the transport phenomena, i.e. Newton’s law of viscosity and Fourier’s heat conduction law. These equations are given in the variables  $(T, \varrho, \mathbf{v})$  or  $(T, p, \mathbf{v})$ .

Replacing (2.29) into (2.2) one obtains the Navier–Stokes equation

$$\varrho \dot{\mathbf{v}} = -\nabla p + \left[ \frac{\mu^{\text{Vol}} - \mu^{\text{Sh}}}{3} (\nabla \cdot \mathbf{v}) \mathbf{1} + \frac{\mu^{\text{Sh}}}{2} (\mathbf{v} \otimes \nabla + \nabla \otimes \mathbf{v}) \right] \cdot \nabla.$$

Since

$$\varrho \dot{u} = \varrho c_v \dot{T} - \left( T \frac{\beta_p}{\chi_T} - p \right) \frac{1}{\varrho} \dot{\varrho} \stackrel{(2.1)}{=} \varrho c_v \dot{T} + \left( T \frac{\beta_p}{\chi_T} - p \right) \nabla \cdot \mathbf{v}$$

and applying (2.28) the balance of internal energy can be given as

$$\begin{aligned} \varrho c_v \dot{T} &= -\nabla \cdot (\lambda \nabla T) - T \frac{\beta_p}{\chi_T} \nabla \cdot \mathbf{v} \\ &\quad + \left[ \frac{\mu^{\text{Vol}} - \mu^{\text{Sh}}}{3} (\nabla \cdot \mathbf{v}) \mathbf{1} + \frac{\mu^{\text{Sh}}}{2} (\mathbf{v} \otimes \nabla + \nabla \otimes \mathbf{v}) \right] : (\mathbf{v} \otimes \nabla). \end{aligned}$$

Let us now express  $\nabla \cdot \mathbf{v}$  from (2.1) in the variables  $(T, p)$ , i.e.

$$\nabla \cdot \mathbf{v} = -\frac{1}{\varrho} \dot{\varrho} = \beta_p \dot{T} - \chi_T \dot{p}$$

then

$$\begin{aligned} \varrho \left( c_v + \frac{T \beta_p^2}{\varrho \chi_T} \right) \dot{T} &= -\nabla \cdot (\lambda \nabla T) + \beta_p T \dot{p} \\ &\quad + \left[ \frac{\mu^{\text{Vol}} - \mu^{\text{Sh}}}{3} (\nabla \cdot \mathbf{v}) \mathbf{1} + \frac{\mu^{\text{Sh}}}{2} (\mathbf{v} \otimes \nabla + \nabla \otimes \mathbf{v}) \right] : (\mathbf{v} \otimes \nabla), \end{aligned}$$

where on the left hand side the isobaric specific heat capacity is recognized, i.e.,

$$\begin{aligned} \varrho c_p \dot{T} &= -\nabla \cdot (\lambda \nabla T) + \beta_p T \dot{p} \\ &\quad + \left[ \frac{\mu^{\text{Vol}} - \mu^{\text{Sh}}}{3} (\nabla \cdot \mathbf{v}) \mathbf{1} + \frac{\mu^{\text{Sh}}}{2} (\mathbf{v} \otimes \nabla + \nabla \otimes \mathbf{v}) \right] : (\mathbf{v} \otimes \nabla). \end{aligned}$$

Our previous calculations have pointed out that the transport coefficients  $\lambda$ ,  $\mu^{\text{Vol}}$ , and  $\mu^{\text{Sh}}$  can depend on the state variables and on their gradients, too. According to Noll's material frame-indifference [18], we exclude velocity dependence. The thermostatic constitutions provide the opportunity to transform energy and density dependence into temperature and pressure dependence, i.e. the functional relationships

$$\begin{aligned}\lambda &= \lambda(T, \nabla T, p, \nabla p, \mathbf{v} \otimes \nabla), \\ \mu^{\text{Vol}} &= \mu^{\text{Vol}}(T, \nabla T, p, \nabla p, \mathbf{v} \otimes \nabla), \\ \mu^{\text{Sh}} &= \mu^{\text{Sh}}(T, \nabla T, p, \nabla p, \mathbf{v} \otimes \nabla)\end{aligned}$$

can be assumed on the transport coefficients.

This gradient dependency can significantly affect such phenomena, where sudden changes can appear. For example, the piston effect is induced by fast thermal expansion in the hydraulic boundary layer, resulting in a pressure wave coupled to the temperature field. Since this phenomenon requires particular fluid properties, it is most probable nearby the critical point [19], where the material properties and transport properties are notably sensitive to pressure and temperature. This is a challenging task for thermodynamic modeling and numerical simulations. However, according to acoustic wave propagation, large gradients in the temperature and pressure fields occur.

Another example is the propagation of shock waves for which a steep change occurs between the two sides of the wave. Here, the presence of nonlinear transport coefficients essentially influences the outcome. Adding that the shock wave thickness is usually around the same magnitude as the mean free path [20], the presence of steep gradients in the thermodynamic model becomes crucial.

Shock waves are often investigated for rarefied gases, which are low-pressure gas states, and mass density dependence is crucial for transport properties. Besides, both thermal and fluid parts must be extended and coupled in a particular way on the level of the constitutive equations, i.e. for that situation, the NSF theory is not applicable [21, 22]. Additionally, since the transport coefficients are not independent of each other [22], it is of great importance to investigate the corresponding methodologies from closer, allowing further possibilities. In this respect, it would also be interesting to investigate how kinetic theory could implement such properties. For example, [23] shows a particular example, when the transport coefficients depend on the velocity gradient and that result is found on kinetic grounds. Although it is not a necessary property of the model, it could improve the agreement between theory and experimental data.

However, measuring gradient dependency is a non-trivial task. When one observes size-dependent material coefficients [24], probably an evident manifestation of gradient dependency is identified. This requires further investigation as it is not straightforward how to clearly separate the effects from each other.

That type of nonlinearity is not yet investigated from a numerical point of view. It stands as an open question, how to treat them compatibly with space-time aspects and how it influences the dissipation and dispersion errors in a scheme.

More importantly, how to construct a scheme that preserves the system's total energy in the same way as symplectic integrators work.

As a closing remark, we would like to emphasize that the  $\nabla T$  dependence of the thermal conductivity is not equivalent to the heat flux dependence, which appears in some recent studies [25], not even in Fourier's case. For a non-Fourier equation-such as the Maxwell–Cattaneo–Vernotte equation-the heat flux dependence could be another interpretation for the  $\nabla T$  dependence.

Overall, the present study is devoted to open further discussion and research on the transport coefficients as these quantities are the most crucial part of any modeling task.

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**ГРАДИЈЕНТНО ЗАВИСНИ ТРАНСПОРТНИ КОЕФИЦИЈЕНТИ  
У НАВИЈЕР-СТОКС-ФУРИЈЕОВОМ СИСТЕМУ**

РЕЗИМЕ. У инжењерској пракси, Њутнов закон вискозности и Фуријеов закон провођења топлоте се примењују у описивању термомеханичких процеса у флуидима. И поред њихове успешне примене, постоје нејасни и недовољно истражени детаљи на које је делимично одговорено у овом раду применом метода иреверзибилне термодинамике. Лиуов поступак је примењен за извођење стопе продукције ентропије, у којој је позитивна дефинитност обезбеђена путем линеарних Онзагерових једначина, а које управо представљају Њутнов закон вискозности и Фуријеов закон провођења топлоте. Прорачуни указују да теоријски одређени транспортни коефицијенти (топлотна проводљивост и вискозност) могу зависити и од градијената променљивих стања. Ова градијентна зависност транспортних коефицијената може имати значајан утицај на моделирање појава као што су заваривање, клипни ефекат или ударни таласи.

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