archives
of thermodynamics
Vol. **43**(2022), No. 2, 119–127
DOI: 10.24425/ather.2022.141981

Classical irreversible thermodynamics versus extended irreversible thermodynamics. The role of the continuity equation

CARMINE DI NUCCI*
DANIELE CELLI
PIERA FISCHIONE
DAVIDE PASQUALI

Environmental and Maritime Hydraulic Laboratory (LIAM),
Civil, Construction-Architectural and Environmental Engineering
Department (DICEAA), University of L'Aquila,
Piazzale Ernesto Pontieri 1, Monteluco di Roio, 67100 L'Aquila, Italy

Abstract This brief note focuses on a simple fluid, i.e., a homogeneous, chemically inert, and electrically neutral fluid, for which, in the linear non-equilibrium regime, the thermodynamic state is expressed by a relation between pressure, temperature, and density. The approach based on the elementary scales is used to check the validity range of both the classical irreversible thermodynamics and the extended irreversible thermodynamics. The achieved result reveals that the classical irreversible thermodynamics fails in providing an adequate response when the mechanical solicitations exceed limit values.

Keywords: Classical irreversible thermodynamics; Extended irreversible thermodynamics; Elementary scales method; Discrete approach

*Corresponding Author. Email: carmine.dinucci@univaq.it

Nomenclature

b	–	generic field function
$b(\boldsymbol{r}, t)$	–	spatial (Eulerian) field
$b(\boldsymbol{r}_0, t)$	–	material (Lagrangian) field
$\|dt\|$	–	elementary time scale
$\|d\boldsymbol{r}\|$	–	elementary spatial scale
$\frac{D}{Dt}b(\boldsymbol{r}, t) = \frac{\partial}{\partial t}b(\boldsymbol{r}, t) + \nabla b(\boldsymbol{r}, t) \cdot \boldsymbol{v}(\boldsymbol{r}, t)$	–	material derivative
$\underline{\boldsymbol{J}}(\boldsymbol{r}_0, t) = \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{r}_0}$	–	Jacobian of the coordinate transformation
$J(\boldsymbol{r}_0, t) = \det\left(\underline{\boldsymbol{J}}(\boldsymbol{r}_0, t)\right)$	–	Jacobian determinant
l	–	molecular length
p	–	thermodynamic pressure
$\boldsymbol{r}$	–	Eulerian coordinates
t	–	time variable
T	–	absolute temperature
t_r	–	relaxation time
$\boldsymbol{v}$	–	velocity
V_{t_0}	–	material volume (with constant mass) at the initial time $t = t_0$
V_t	–	material volume at the generic time t
∇b	–	gradient of b
$\nabla \boldsymbol{v}$	–	velocity gradient tensor
$\|\nabla \boldsymbol{v}\, dt\|$	–	dimensionless number

Greek symbols

$\alpha = \alpha(p, T)$	–	thermal expansion coefficient
$\varepsilon = \varepsilon(p, T)$	–	bulk modulus of elasticity
ρ	–	density

Acronyms

CIT	–	classical irreversible thermomechanics
EIT	–	extended irreversible thermodynamics
LTE	–	local thermodynamic equilibrium
REV	–	representative elementary volume

1 Introduction

In agreement with the continuum model of the fluid mechanics, the generic field function b (for instance density ρ, thermodynamic pressure p, absolute temperature T, etc.) is a regular function of both space and time [1]. The space continuity is connected to the continuum hypothesis: the fluid is modeled as a continuum medium, where the single fluid particles are in one-to-one correspondence with the points of the Euclidean space. The minimum volume on which to assess the (average) physical properties of the continuum is the representative elementary volume (REV) dV. The use of the method of homogenization implies that the REV must be *large* compared to the fluid molecular size and *small* compared to the size of the flow domain [2]. Therefore, the space continuity means that

$$\frac{l}{|d\boldsymbol{r}|} \ll 1, \tag{1}$$

where l is a molecular length, $|d\boldsymbol{r}|$ the elementary spatial scale. $|d\boldsymbol{r}|$ can be assumed proportional to the scale of the generic field function gradient [1]:

$$|d\boldsymbol{r}| \propto \left|\frac{b}{\nabla b}\right|. \tag{2}$$

As the term $|\nabla b|$ increases, i.e., the mechanical and/or thermal solicitations increase, then $|d\boldsymbol{r}|$ decreases. The lower limit value must be in accordance with the relationship (1). Beyond this lower limit, the continuum model is not suitable for describing the phenomena.

In classical irreversible thermomechanics (CIT), the time continuity requires that

$$\frac{t_r}{|dt|} \ll 1, \tag{3}$$

where t_r is the relaxation time, i.e., the time it takes to restore a local thermodynamic equilibrium (LTE) condition from a local thermodynamic non-equilibrium condition, $|dt|$ the elementary time scale [3]. For long relaxation time and/or for short elementary time scale, the LTE is invalid, and $\frac{t_r}{|dt|} \sim 1$. These kinds of phenomena can be described by the extended irreversible thermodynamics (EIT) generalizing the classical thermodynamics relationships and the constitutive equations (a review of this topic can be found in [4–6]). It should be stressed that the study approach based on the elementary scales allows to extend and refine the range of applicability of the classical irreversible thermodynamics. In [7], the elementary time scale is used to define a turbulence model able to describe the energy dissipation in shock waves; in [3] a method based on the elementary scales is employed to remove the heat conduction paradox concerning the infinite speed of signal diffusion in the Fourier theory (Fourier paradox). The choice of the elementary time scale $|dt|$ is not arbitrary. As outlined in the following section, the constrain that the continuum model imposes to $|dt|$ can be linked to the velocity gradient tensor $\|\nabla \boldsymbol{v}\|$ which, in turn, is linked to the mechanical solicitations. This result is related to the study of the continuity equation. For the sake of clarity, this note is focused on a simple fluid, i.e., a homogeneous fluid, chemically inert, and electrically neutral, whose thermodynamic state, in the linear non-equilibrium regime, is expressed by a relation between pressure, temperature and density [8].

2 Continuity equation

The mass conservation principle ensures that

$$\int\limits_{V_{t_0}} \rho\left(\boldsymbol{r}_0, t_0\right)\, dV_{t_0} = \int\limits_{V_t} \rho(\boldsymbol{r}, t)\, dV_t, \tag{4}$$

where V_{t_0} is the material volume (with constant mass) at the initial time $t = t_0$; V_t is the material volume at the generic time t; $\boldsymbol{r}$ and t are the Eulerian coordinates, with $\boldsymbol{r}$ – the space variable and t – the time variable; $\boldsymbol{r}_0$ and t are the material (Lagrangian) coordinates; $\rho(\boldsymbol{r}, t)$ is the spatial (Eulerian) density field. The mapping from $\boldsymbol{r}_0$ to $\boldsymbol{r}$, given by the continuous and invertible function

$$\boldsymbol{r}_0 = \boldsymbol{r}_0(\boldsymbol{r}, t), \tag{5}$$

can be used to express the connection between the spatial field $b(\boldsymbol{r}, t)$ and the corresponding material (Lagrangian) field $b(\boldsymbol{r}_0, t)$ as

$$b\left(\boldsymbol{r}_0, t\right) = b\left(\boldsymbol{r}_0(\boldsymbol{r}, t), t\right) = b(\boldsymbol{r}, t). \tag{6}$$

According to Eq. (6), it follows that

$$\frac{d}{dt} b\left(\boldsymbol{r}_0, t\right) = \frac{D}{Dt} b(\boldsymbol{r}, t), \tag{7}$$

where $\dfrac{D}{Dt} b(\boldsymbol{r}, t) = \dfrac{\partial}{\partial t} b(\boldsymbol{r}, t) + \nabla b(\boldsymbol{r}, t) \cdot \boldsymbol{v}(\boldsymbol{r}, t)$ is the material derivative, with $\boldsymbol{v}(\boldsymbol{r}, t)$ the spatial velocity field.

The mapping from $\boldsymbol{r}_0$ to $\boldsymbol{r}$ can be viewed as a coordinate transformation, where the Jacobian of the transformation $\underline{\boldsymbol{J}}$ is given as

$$\underline{\boldsymbol{J}}\left(\boldsymbol{r}_0, t\right) = \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{r}_0}\,. \tag{8}$$

The Jacobian determinant $J(\boldsymbol{r}_0,t) = \det\left(\underline{\boldsymbol{J}}(\boldsymbol{r}_0,t)\right)$ allows expressing the connection between dV_{t_0} and dV_t as

$$dV_t = J\,dV_{t_0}. \tag{9}$$

According to Eq. (9), Eq. (4) becomes:

$$\int\limits_{V_{t_0}} \rho\left(\boldsymbol{r}_0,t_0\right)dV_{t_0} = \int\limits_{V_{t_0}} \rho\left(\boldsymbol{r}_0,t\right)J\left(\boldsymbol{r}_0,t\right)dV_{t_0} \tag{10}$$

from which it follows that

$$\frac{1}{J\left(\boldsymbol{r}_0,t\right)}\rho\left(\boldsymbol{r}_0,t_0\right) = \rho\left(\boldsymbol{r}_0,t\right). \tag{11}$$

Equation (11) can be derived with respect to time:

$$\frac{-\rho\left(\boldsymbol{r}_0,t_0\right)}{\left[J\left(\boldsymbol{r}_0,t\right)\right]^2}\frac{dJ\left(\boldsymbol{r}_0,t\right)}{dt} = \frac{d\rho\left(\boldsymbol{r}_0,t\right)}{dt}. \tag{12}$$

Using the Euler formula [9]

$$\frac{1}{J\left(\boldsymbol{r}_0,t\right)}\frac{dJ\left(\boldsymbol{r}_0,t\right)}{dt} = \nabla\cdot\boldsymbol{v}(\boldsymbol{r},t). \tag{13}$$

Eq. (12) reduces to the continuity equation

$$\begin{aligned}\frac{-\rho\left(\boldsymbol{r}_0,t_0\right)}{J\left(\boldsymbol{r}_0,t\right)}\frac{1}{J\left(\boldsymbol{r}_0,t\right)}\frac{dJ\left(\boldsymbol{r}_0,t\right)}{dt} &= -\rho\left(\boldsymbol{r}_0,t\right)\nabla\cdot\boldsymbol{v}(\boldsymbol{r},t)\\ &= -\rho(\boldsymbol{r},t)\nabla\cdot\boldsymbol{v}(\boldsymbol{r},t) = \frac{D\rho(\boldsymbol{r},t)}{Dt},\end{aligned} \tag{14}$$

being $\dfrac{d\rho\left(\boldsymbol{r}_0,t\right)}{dt} = \dfrac{D\rho(\boldsymbol{r},t)}{Dt}$, $\rho\left(\boldsymbol{r}_0,t\right) = \rho\left(\boldsymbol{r}_0(\boldsymbol{r},t),t\right) = \rho(\boldsymbol{r},t)$. In explicit form, the continuity equation is given by the well-known equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}) = 0. \tag{15}$$

Within the framework of the continuum model, the above procedure is exact (without approximations). On the other hand, the continuity equation can be deduced using a second approach [3, 10]. Setting

$$\boldsymbol{r}^* = \boldsymbol{r} + d\boldsymbol{r} = \boldsymbol{r} + \boldsymbol{v}(\boldsymbol{r},t)\,dt \tag{16}$$

the Jacobian tensor $\underline{\boldsymbol{J}}$ is given as

$$\underline{\boldsymbol{J}} = \frac{\partial \boldsymbol{r}^*}{\partial \boldsymbol{r}} = \nabla \boldsymbol{r}^* = \underline{\boldsymbol{I}} + \nabla \boldsymbol{v}\, dt. \tag{17}$$

Defining $dV = dV(\boldsymbol{r}, t)$ and $dV^* = dV(\boldsymbol{r}^*, t^*) = dV(\boldsymbol{r} + d\boldsymbol{r}, t + dt)$, with $t^* = t + dt$, the relationship between dV and dV^* is expressed by

$$dV^* = J\, dV, \tag{18}$$

where the Jacobian determinant reads as

$$J = \det \underline{\boldsymbol{J}} = \det\left(\underline{\boldsymbol{I}} + \nabla \boldsymbol{v}\, dt\right). \tag{19}$$

According to this, the mass conservation principle can be expressed as

$$\rho\, dV = \rho^*\, dV^*, \tag{20}$$

where:

$$\rho = \rho(\boldsymbol{r}, t), \tag{21}$$

$$\begin{aligned} \rho^*(\boldsymbol{r}^*, t^*) &= \rho(\boldsymbol{r} + d\boldsymbol{r}, t + dt) \\ &= \rho(\boldsymbol{r}, t) + \frac{\partial \rho(\boldsymbol{r}, t)}{\partial t} dt + \frac{\partial \rho(\boldsymbol{r}, t)}{\partial \boldsymbol{r}} \cdot d\boldsymbol{r} \\ &= \rho + \frac{\partial \rho}{\partial t}\, dt + \nabla \rho \cdot d\boldsymbol{r} \\ &= \rho + \frac{\partial \rho}{\partial t}\, dt + \nabla \rho \cdot \boldsymbol{v}\, dt. \end{aligned} \tag{22}$$

If $\|\nabla \boldsymbol{v}\, dt\| \ll 1$, Eq. (19) can be approximated as [10,11]

$$J = 1 + \nabla \cdot \boldsymbol{v}\, dt \tag{23}$$

and Eq. (20) reads as

$$\rho\, dV = \left(\rho + \frac{\partial \rho}{\partial t}\, dt + \nabla \rho \cdot \boldsymbol{v}\, dt\right)(1 + \nabla \cdot \boldsymbol{v}\, dt)\, dV. \tag{24}$$

In the case in which higher-order infinitesimal can be neglected, Eq. (24) reduces to Eq. (15).

It is possible to observe that this second procedure is not exact, and it introduces some approximations. The comparison between the two procedures implies that for every $\nabla \boldsymbol{v}$ there exists dt such that $\|\nabla \boldsymbol{v}\, dt\| \ll 1$. This result is intrinsic to the continuum model: within the framework of the continuum model, the dimensionless number $\|\nabla \boldsymbol{v}\, dt\|$ is always evanescent (the larger $\|\nabla \boldsymbol{v}\|$, the lower $|dt|$); accordingly, the elementary time scale $|dt|$ is linked to the velocity gradient $\|\nabla \boldsymbol{v}\|$, which, in turn, is linked to mechanical solicitations. When the mechanical solicitations overcome the limit values, the LTE assumption is not valid, and the CIT is not suitable for describing these kinds of phenomena: under these conditions, $\dfrac{t_r}{|dt|} \sim 1$, and the EIT can be used.

It should be stressed that, as $\|\nabla \boldsymbol{v}\, dt\| \ll 1$, then $\det(\underline{\boldsymbol{I}} + \nabla \boldsymbol{v}\, dt) = 1 + \nabla \cdot \boldsymbol{v}\, dt$ is close to 1 and, therefore, also the dimensionless number $|\nabla \cdot \boldsymbol{v}\, dt|$ is always evanescent, $|\nabla \cdot \boldsymbol{v}\, dt| \ll 1$ [3]. Formally, the continuum model assures that for every $\nabla \cdot \boldsymbol{v}$ there exist dt such that $|\nabla \cdot \boldsymbol{v}\, dt| \ll 1$. This result can be used to define the REV scale in CIT. In CIT, the differential state equation reads as [12]

$$\frac{-1}{\rho}\, d\rho = \frac{-1}{\varepsilon}\, dp + \alpha\, dT, \tag{25}$$

where $\varepsilon = \varepsilon(p, T)$ is the bulk modulus of elasticity and $\alpha = \alpha(p, T)$ is the thermal expansion coefficient. Using the conservation continuity equation

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \boldsymbol{v} = 0 \tag{26}$$

the following relationship holds:

$$\frac{-1}{\rho}\, d\rho = \nabla \cdot \boldsymbol{v}\, dt \tag{27}$$

and Eq. (25) reads as

$$\nabla \cdot \boldsymbol{v}\, dt = \frac{-1}{\varepsilon}\, dp + \alpha\, dT. \tag{28}$$

As $|\nabla \cdot \boldsymbol{v}\, dt| \ll 1$, then $\dfrac{1}{\varepsilon}|dp| \sim \alpha |dT|$ or (equivalently) $\dfrac{1}{\varepsilon}|\nabla p| \sim \alpha |\nabla T|$. In agreement with this result, that is intrinsic to CIT, when the thermal solicitation is predominant, setting in Eq. (2) $b = p$ and $|\nabla p| \sim \alpha\varepsilon |\nabla T|$, the REV scale can be expressed as

$$|d\boldsymbol{r}| \propto \frac{1}{\alpha\varepsilon} \left| \frac{p}{\nabla T} \right|. \tag{29}$$

On the other hand, when the mechanical solicitation plays a predominant role, setting in Eq. (2) $b = T$ and $|\nabla T| \sim \dfrac{1}{\alpha\varepsilon}|\nabla p|$, the REV scale can be characterized as

$$|d\boldsymbol{r}| \propto \alpha\varepsilon \left|\frac{T}{\nabla p}\right|. \tag{30}$$

3 Conclusions

The continuum model of the fluid mechanics involves the elementary spatial scale $|d\boldsymbol{r}|$ and the elementary temporal scale $|dt|$.

On the one hand, $|d\boldsymbol{r}|$ is linked to the scale of the gradient of the generic field function (see Eq. (2)). When thermal and/or mechanical solicitations overcome the limit values, the continuum model is not suitable for describing the phenomena. In classical irreversible thermodynamics, $|d\boldsymbol{r}|$ can be assumed proportional to $|\nabla p|$ or $|\nabla T|$, depending on what solicitation (mechanical or thermal) is predominant (see Eqs. (29)–(30)).

On the other hand, $|dt|$ is linked to the mechanical solicitation through the velocity gradient tensor. The continuum model assures that for every $\nabla\boldsymbol{v}$ there exists dt such that $\|\nabla\boldsymbol{v}\,dt\| \ll 1$ (as $\|\nabla\boldsymbol{v}\|$ increases, then $|dt|$ decreases, and the dimensionless number $\|\nabla\boldsymbol{v}\,dt\|$ is always evanescent); for every $\nabla\cdot\boldsymbol{v}$ there exist dt such that $|\nabla\cdot\boldsymbol{v}\,dt| \ll 1$ (as $\|\nabla\boldsymbol{v}\,dt\| \ll 1$, then also the dimensionless number $|\nabla\cdot\boldsymbol{v}\,dt|$ is always evanescent). According to these results, which are intrinsic to the continuity equation, when the mechanical solicitations overcome the limit values, the local thermodynamic equilibrium assumption is not valid, and $\dfrac{t_r}{|dt|} \sim 1$. Then, the classical irreversible thermodynamics is not suitable for describing these kinds of phenomena. Under these conditions, the extended irreversible thermodynamics can be used. It should be stressed that the study approach based on the elementary scales allows to extend and refine the range of applicability of the classical irreversible thermodynamics.

Received 19 May 2022

References

[1] Gad-el-Hak M.: *The fluid mechanics of microdevices-the Freeman scholar lecture.* J. Fluids Eng. **121**(1999), 1, 5–33.

[2] Auriault J.-L.: *Homogenization theory applied to porous media.* Poromechanics **3**(2005), 113–120.

[3] Di Nucci C., Celli D., Fischione P., Pasquali D.: *Elementary scales and the lack of Fourier paradox for Fourier fluids.* Meccanica **57**(2022), 251–254.

[4] Jou D., Casas-Vázquez J., Lebon G.: *Extended Irreversible Thermodynamics revisited (1988–98).* Rep. Prog. Phys. **62**(1999), 7, 1035–1142.

[5] Lenarczyk M., Domański R.: *Investigation of non-Fourier thermal waves interaction in a solid material.* Arch. Thermodyn. **40**(2019), 1, 115–126.

[6] Othman M.I.A., Abouelregal A.E.E.: *The effect of pulsed laser radiation on a thermoviscoelastic semi-infinite solid under two-temperature theory.* Arch. Thermodyn. **38**(2017), 3, 77–99.

[7] Di Nucci C., Pasquali D., Celli D., Pasculli A., Fischione P., Di Risio M.: *Turbulent bulk viscosity.* Eur. J. Mech. B-Fluid. **84**(2020), 446–454.

[8] Durst F.: *Fluid Mechanics: An Introduction to the Theory of Fluid Flows.* Springer-Verlag, Berlin – Heidelberg 2008.

[9] Frost W., Moulden T.H. (Eds.): *Handbook of Turbulence: Vol. 1 Fundamentals and Applications.* Plenum Press, New York – London 1977.

[10] Gallavotti G.: *Foundations of Fluid Dynamics.* Springer-Verlag, Berlin – Heidelberg 2002.

[11] Petersen K.B., Pedersen M.S.: *The Matrix Cookbook.* Tech. Univ. of Denmark, 2008.

[12] Panton R.: *Incompressible Flow.* John Wiley & Sons, Hoboken 2013.