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# A note on thermodynamic restriction on turbulence modelling

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**Abstract**

Within the framework of rational thermodynamics set forth by Truesdell and Toupin [In: S. Flügge, C. Truesdell (Eds.), Handbuch der Physik III/1, Springer, Berlin, 1960], and Coleman and Noll [Arch. Rational Mech. Anal. 13 (1963) 167–178], among others, we study thermodynamic restriction on turbulence modelling. First, we show that the turbulent kinetic energy equation is a direct consequence of the first law of thermodynamics, and in view of the second law of thermodynamics the turbulent dissipation rate is in nature a thermodynamic internal variable. Second, we show that the principle of entropy growth expressed in the forms of the Clausius–Duhem and the Clausius–Planck inequalities, places a restriction on turbulence modelling, wherein the turbulent dissipation rate as a thermodynamic internal variable plays a key role in ensuring the modelling adopted to be thermodynamically admissible. 

*Keywords:* Clausius–Duhem inequality; Internal dissipation; Turbulent dissipation rate; Turbulence modelling; Thermodynamic constraint

## 1. Introduction

It is well known that the Clausius–Duhem inequality put forth by Truesdell and Toupin (1960) as a general form of the principle of entropy growth for continuous media has been widely applied in modern continuum mechanics for the past 40 years (cf. Truesdell, 1984). The idea that the Clausius–Duhem inequality should be interpreted as an identical restriction on constitutive relations was first suggested and applied by Coleman and Noll (1963) in their studies of elastic materials with heat conduction and viscosity. In a fundamental research on thermodynamics of simple materials, Coleman (1964) took the Clausius–Duhem inequality to be the expression of the principle of entropy growth and constructed a systematic method for reducing constitutive equations to forms compatible with thermodynamics. The researches carried out by Coleman (1964) and Coleman and Noll (1963) in the early 1960s show that the Clausius–Duhem inequality severely restricts the behavior of the response functionals, namely, the constitutive equations, for the stress, the heat flux, the internal energy, the entropy, and the free energy. Since then, a great deal of follow-up researches on this line set forth by Coleman and Noll have been witnessed in the literature of the many branches of continuum mechanics (cf. e.g., Eringen and Maugin, 1990; Huang and Batra, 1996).

Recently, Sadiki et al. (1999) and Sadiki et al. (2000), among others, investigated the thermodynamic constraints on closure models for turbulence in the context of extended thermodynamics; readers are referred to their work for a review on various constraints on turbulence modelling. They demonstrated in their papers that many non-linear and anisotropic turbulence models are in fact not thermodynamically admissible, and they further showed that the so-called "realizability constraints" of Schumann (1977) are contained in the second law of thermodynamics as one among other mathematical conditions derived in exploiting the entropy inequality. It is noticed that in their approach, the results obtained rely on an introduced turbulent Helmholtz free energy $\psi^{\mathrm{T}}$, which is assumed to take the following form:

$$\psi^{\mathrm{T}} = K\left(\ln\frac{C_0^{\mathrm{T}}\varepsilon}{K} + \frac{1}{2}\alpha\varepsilon^2\overline{D}_{ij}\overline{D}_{ij} + b(\varepsilon_{,i})^2 + A_0\right), \tag{1}$$

where $\alpha$, $b$, $A_0$ and $C_0^{\mathrm{T}}$ are constants, $K$ is the turbulent kinetic energy, $\varepsilon$ is the turbulent dissipation rate, $\bar{\mathbf{v}}$ is the mean velocity, and $\overline{\mathbf{D}} = \frac{1}{2}(\operatorname{grad}\bar{\mathbf{v}} + (\operatorname{grad}\bar{\mathbf{v}})^{\mathrm{T}})$.

Turbulence is regarded as a continuum phenomenon which can be described within the framework of continuum mechanics, and in fact the turbulent flow is a thermodynamic process. Then, under what conditions the constitutive equations proposed for solving the Reynolds-averaged Navier–Stokes equations are compatible with the principle of entropy growth? In fact, to require a constitutive equation to be thermodynamically compatible is to impose restrictions upon it. In this note, we shall follow the line of rational

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thermodyanmics, to study the relationships of the second law of thermodynamics with turbulence modelling. It will be seen that the turbulent dissipation rate is in nature a thermodynamic internal variable in view of the second law of thermodynamics, and the Clausius–Planck inequality, which is a reduced form of the Clausius–Duhem inequality when the temperature field is homogeneous, places a restriction on modelling the turbulent flows of an incompressible Navier–Stokes fluid.

## 2. Internal dissipation and the Clausius–Planck inequality

In continuum mechanics, the laws assumed to hold from the outset for materials of simple traction are, in an inertial frame,

$$\dot{\varrho} + \varrho \operatorname{div} \mathbf{v} = 0, \tag{2}$$

$$\varrho \dot{\mathbf{v}} = \operatorname{div} \mathbf{T} + \varrho \mathbf{b}, \tag{3}$$

$$\mathbf{T} = \mathbf{T}^{\mathrm{T}}, \tag{4}$$

$$\varrho \dot{e} = \operatorname{tr}(\mathbf{TD}) + \operatorname{div} \mathbf{h} + \varrho s, \tag{5}$$

where $\varrho$ is the mass density, $\mathbf{v}$ is the velocity, $\mathbf{T}$ is the Cauchy stress, $e$ is the specific internal energy, $\mathbf{D}$ is the stretching tensor ($2\mathbf{D} = \operatorname{grad} \mathbf{v} + (\operatorname{grad} \mathbf{v})^{\mathrm{T}}$), $s$ is the supply of heating, $\mathbf{b}$ is the body force density, $\mathbf{h}$ is the heat flux, and the dot represents the material time derivative.

Here, Eq. (5) (the Fourier–Kirchhoff–Neumann equation) is the local form of the first law of thermodynamics, i.e., the energy balance equation. Now with the specific free energy $\Psi$ defined by

$$\Psi := e - \eta\theta, \tag{6}$$

where $\theta$ is the absolute temperature ($\theta > 0$), and $\eta$ is the specific entropy, we have the local expression of the Clausius–Duhem inequality (cf. Truesdell and Noll, 1965; Truesdell, 1984)

$$\varrho\theta\dot{\eta} \geqslant \theta \operatorname{div}\left(\frac{\mathbf{h}}{\theta}\right) + \varrho s, \tag{7}$$

equivalently,

$$\varrho(\theta\dot{\eta} - \dot{e}) + \operatorname{tr}(\mathbf{TD}) + \frac{\mathbf{h} \cdot \operatorname{grad} \theta}{\theta} \geqslant 0; \tag{8}$$

also, the internal dissipation $\delta$ is defined as

$$\delta := \varrho\theta\dot{\eta} - (\operatorname{div} \mathbf{h} + \varrho s), \tag{9}$$

equivalently,

$$\delta = \operatorname{tr}(\mathbf{TD}) - \varrho(\dot{\Psi} + \eta\dot{\theta}) = \operatorname{tr}(\mathbf{TD}) - \varrho(\dot{e} - \theta\dot{\eta}), \tag{10}$$

which denotes the amount by which the increase of entropy times the temperature exceeds the local heating.

If the temperature is homogeneous, the Clausius–Duhem inequality (7) reduces to the Clausius–Planck inequality

$$\varrho\theta\dot{\eta} \geqslant \operatorname{div} \mathbf{h} + \varrho s. \tag{11}$$

It is evident from Eqs. (9) and (11) that the necessary and sufficient condition for the Clausius–Planck inequality is

$$\delta \geqslant 0. \tag{12}$$

Now consider the Navier–Stokes fluid (cf. Coleman and Noll, 1963)

$$\mathbf{T} = -p\mathbf{1} + \lambda \operatorname{tr}(\mathbf{D})\mathbf{1} + 2\mu\mathbf{D}, \tag{13}$$

where $p$ is the pressure, $\mathbf{1}$ is the unit tensor, $\mu$ is the shear viscosity, and $\lambda + \frac{2}{3}\mu$ is the bulk viscosity. Note that

$$e = e(v, \eta), \quad p = -\partial_v e, \quad \theta = \partial_\eta e, \tag{14}$$

where $v = 1/\varrho$.

By Eq. (10), the internal dissipation reads

$$\delta = \lambda(\operatorname{tr} \mathbf{D})^2 + 2\mu \operatorname{tr}(\mathbf{D}^2). \tag{15}$$

From Eqs. (12) and (15), noting $(\operatorname{tr} \mathbf{D})^2 \leqslant 3 \operatorname{tr} \mathbf{D}^2$, follow readily the Duhem–Stokes inequalities:

$$\mu \geqslant 0, \quad 3\lambda + 2\mu \geqslant 0, \tag{16}$$

which is the necessary and sufficient condition for non-negativeness of the internal dissipation in this case.

Moreover, if the fluid is incompressible, then the Duhem–Stokes inequalities (16) simply become

$$\mu \geqslant 0. \tag{17}$$

Hence, we see that for an incompressible Navier–Stokes fluid, where the Cauchy stress takes the form

$$\mathbf{T} = -p\mathbf{1} + 2\mu\mathbf{D}, \tag{18}$$

the viscosity $\mu \geqslant 0$ is merely a thermodynamic restriction on the fluid itself. In the following, we shall show that in fact the Clausius–Planck inequality, or equivalently as seen, the non-negativeness of the internal dissipation, imposes constraints upon turbulence modelling. We shall return to this point later.

## 3. Thermodynamic restriction on turbulence modelling

Here, we consider an incompressible Navier–Stokes fluid with constant mass density $\varrho$ and viscosity $\mu$. So from Eqs. (2)–(5), it follows that

$$\operatorname{div} \mathbf{v} = 0, \tag{19}$$

$$\varrho \dot{\mathbf{v}} = \operatorname{div} \mathbf{T} + \varrho \mathbf{b}, \tag{20}$$

$$\varrho \dot{e} = \operatorname{tr}(\mathbf{TD}) + \operatorname{div} \mathbf{h} + \varrho s, \tag{21}$$

where now $\mathbf{T} = -p\mathbf{1} + 2\mu\mathbf{D}$.

Taking the ensemble average on Eqs. (19)–(21), we have

$$\operatorname{div} \bar{\mathbf{v}} = 0, \tag{22}$$

$$\varrho \overset{\circ}{\bar{\mathbf{v}}} = \operatorname{div}(\bar{\mathbf{T}} - \boldsymbol{\tau}) + \varrho \bar{\mathbf{b}}, \tag{23}$$

$$\varrho \dot{\bar{e}} = \operatorname{tr}(\bar{\mathbf{T}}\bar{\mathbf{D}}) + \operatorname{tr}(\overline{\mathbf{T}'\mathbf{D}'}) + \operatorname{div} \bar{\mathbf{h}} + \varrho \bar{s}, \tag{24}$$

where the overbar represents the ensemble average, and the prime $'$ denotes the fluctuation, the $\circ$ stands for the material time derivative associated with mean velocity $\bar{\mathbf{v}}$, $\boldsymbol{\tau} := \varrho\overline{\mathbf{v}' \otimes \mathbf{v}'}$ is the Reynolds stress tensor, and $\mathbf{T}' = -p'\mathbf{1} + 2\mu\mathbf{D}'$, where $2\mathbf{D}' = \operatorname{grad} \mathbf{v}' + (\operatorname{grad} \mathbf{v}')^{\mathrm{T}}$.

We shall derive the turbulent kinetic energy equation directly based on the first law of thermodynamics. To this end, let us consider the global energy balance equation

$$\dot{\mathscr{K}} + \dot{\mathscr{E}} = \mathscr{P} + \mathscr{Q}, \tag{25}$$

where the kinetic energy

$$\mathscr{K} := \frac{1}{2} \int_{\mathscr{B}} \varrho(\mathbf{v} \cdot \mathbf{v}) \, \mathrm{d}V, \tag{26}$$

the heating

$$\mathscr{Q} := \int_{\partial\mathscr{B}} q \, \mathrm{d}S + \int_{\mathscr{B}} \varrho s \, \mathrm{d}V = \int_{\partial\mathscr{B}} \mathbf{h} \cdot \mathbf{n} \, \mathrm{d}S + \int_{\mathscr{B}} \varrho s \, \mathrm{d}V, \tag{27}$$

where $\mathscr{B}$ is the domain occupied by the fluid, $\partial\mathscr{B}$ is the boundary of $\mathscr{B}$, $q = \mathbf{h} \cdot \mathbf{n}$ is the efflux of heating, $\mathbf{n}$ is the normal unit vector; also, the mechanical working

$$\mathscr{P} := \int_{\partial\mathscr{B}} \mathbf{v}\cdot\mathbf{T}\mathbf{n}\,\mathrm{d}S + \int_{\mathscr{B}} \varrho\mathbf{v}\cdot\mathbf{b}\,\mathrm{d}V, \tag{28}$$

and the internal energy

$$\mathscr{E} := \int_{\mathscr{B}} \varrho e\,\mathrm{d}V, \tag{29}$$

where $e$ is the specific internal energy.

The net working is given by

$$\mathscr{P} - \dot{\mathscr{K}} = \int_{\partial\mathscr{B}} \mathbf{v}\cdot\mathbf{T}\mathbf{n}\,\mathrm{d}S + \int_{\mathscr{B}} \varrho\mathbf{v}\cdot\mathbf{b}\,\mathrm{d}V - \int_{\mathscr{B}} \varrho(\mathbf{v}\cdot\dot{\mathbf{v}})\,\mathrm{d}V. \tag{30}$$

Now taking the ensemble average on Eq. (30), noting $\mathrm{div}\,\overline{\mathbf{v}} = \mathrm{div}\,\mathbf{v}' = 0$ and making use of the divergence theorem, a bit involved but straightforward algebra yields

$$\begin{aligned}\overline{\mathscr{P}} - \overline{\dot{\mathscr{K}}} = &\int_{\mathscr{B}} \mathrm{div}(\overline{\mathbf{T}}\,\overline{\mathbf{v}} + \overline{\mathbf{T}'\mathbf{v}'})\,\mathrm{d}V \\ &+ \int_{\mathscr{B}} \varrho\Big\{\overline{\mathbf{v}}\cdot\overline{\mathbf{b}} + \overline{\mathbf{v}'\cdot\mathbf{b}'} - \overline{\mathbf{v}}\cdot\mathring{\overline{\mathbf{v}}} - \overline{\mathbf{v}}\cdot\mathrm{div}(\overline{\mathbf{v}'\otimes\mathbf{v}'}) \\ &- \frac{1}{2}\mathring{\overline{\mathbf{v}'\cdot\mathbf{v}'}} - \overline{\mathbf{v}'\cdot\mathrm{div}(\mathbf{v}'\otimes\mathbf{v}')} - \overline{(\mathbf{v}'\otimes\mathbf{v}')}\cdot\overline{\mathbf{D}}\Big\}\,\mathrm{d}V. \end{aligned} \tag{31}$$

From Eqs. (29) and (25), it follows that

$$\begin{aligned}\overline{\mathscr{E}} &= \int_{\mathscr{B}} \varrho\overline{e}\,\mathrm{d}V = \int_{\mathscr{B}} \varrho(\mathring{\overline{e}} + \overline{(\mathrm{grad}\,e')\cdot\mathbf{v}'})\,\mathrm{d}V \\ &= \overline{\mathscr{P}} - \overline{\dot{\mathscr{K}}} + \overline{\mathscr{Q}}, \end{aligned} \tag{32}$$

where $\overline{\mathscr{Q}} = \int_{\mathscr{B}}(\mathrm{div}\,\overline{\mathbf{h}} + \varrho\overline{s})\,\mathrm{d}V$.

Assuming sufficient smoothness and noting Eq. (31), the local expression of Eq. (32) reads

$$\begin{aligned}\varrho\dot{\overline{e}} &= \varrho\mathring{\overline{e}} + \varrho\overline{(\mathrm{grad}\,e')\cdot\mathbf{v}'} \\ &= (\overline{\mathbf{T}} - \boldsymbol{\tau})\cdot\overline{\mathbf{D}} + \mathrm{div}\,\overline{\mathbf{T}'\mathbf{v}'} + \varrho\overline{\mathbf{b}'\cdot\mathbf{v}'} - \frac{1}{2}\varrho\mathring{\overline{\mathbf{v}'\cdot\mathbf{v}'}} \\ &\quad - \varrho\overline{\mathbf{v}'\cdot\mathrm{div}(\mathbf{v}'\otimes\mathbf{v}')} + \mathrm{div}\,\overline{\mathbf{h}} + \varrho\overline{s}, \end{aligned} \tag{33}$$

where Eq. (23) has been used.

Comparing Eq. (33) with Eq. (24) gives

$$\begin{aligned}&-\boldsymbol{\tau}\cdot\overline{\mathbf{D}} + \mathrm{div}\,\overline{\mathbf{T}'\mathbf{v}'} + \varrho\overline{\mathbf{b}'\cdot\mathbf{v}'} - \frac{1}{2}\varrho\mathring{\overline{\mathbf{v}'\cdot\mathbf{v}'}} - \varrho\overline{\mathbf{v}'\cdot\mathrm{div}(\mathbf{v}'\otimes\mathbf{v}')} \\ &\quad = \overline{\mathbf{T}'\cdot\mathbf{D}'} = \mathrm{tr}(\overline{\mathbf{T}'\mathbf{D}'}). \end{aligned} \tag{34}$$

Eq. (34) is nothing but the turbulent kinetic energy equation of an incompressible fluid under consideration.

Substituting $\mathbf{T}' = -p'\mathbf{1} + 2\mu\mathbf{D}'$ into Eq. (34), we obtain

$$\begin{aligned}\mathring{K} = &-\boldsymbol{\tau}\cdot\overline{\mathbf{D}} + \mathrm{div}\left(-\overline{p'\mathbf{v}'} + 2\mu\overline{\mathbf{D}'\mathbf{v}'} - \frac{1}{2}\varrho\overline{(\mathbf{v}'\cdot\mathbf{v}')\mathbf{v}'}\right) + \varrho\overline{\mathbf{b}'\cdot\mathbf{v}'} - \varepsilon \\ = &-\boldsymbol{\tau}\cdot\overline{\mathbf{D}} + \mathrm{div}\left(-\overline{p'\mathbf{v}'} + \mu\overline{(\mathrm{grad}\,\mathbf{v}' + (\mathrm{grad}\,\mathbf{v}')^{\mathrm{T}})\mathbf{v}'}\right. \\ &\left.-\frac{1}{2}\varrho\overline{(\mathbf{v}'\cdot\mathbf{v}')\mathbf{v}'}\right) + \varrho\overline{\mathbf{b}'\cdot\mathbf{v}'} - \varepsilon, \end{aligned} \tag{35}$$

where $K := \frac{1}{2}\varrho\overline{\mathbf{v}'\cdot\mathbf{v}'} = \frac{1}{2}\mathrm{tr}(\boldsymbol{\tau})$ is the turbulent kinetic energy, and $\varepsilon := 2\mu\overline{\mathbf{D}'\cdot\mathbf{D}'} = \mathrm{tr}(\overline{\mathbf{T}'\mathbf{D}'})$ is the turbulent dissipation rate.

If we set $\mathbf{b}' = \mathbf{0}$, then Eq. (35) reduces to the turbulent kinetic energy equation given in Hinze (1975).

Now we are in a position to show the thermodynamic restriction on the turbulence modelling of an incompressible Navier–Stokes fluid. Let us return to the *necessary and sufficient condition* for the Clausius–Planck inequality (15), which in this case takes the simple form

$$\delta = 2\mu\,\mathrm{tr}(\mathbf{D}^2) \geqslant 0, \tag{36}$$

where $\mu \geqslant 0$, as mentioned earlier, is but a thermodynamic restriction on the incompressible Navier–Stokes fluid per se.

Taking the ensemble average on Eq. (36) of the internal dissipation, we find that

$$\overline{\delta} = 2\mu\,\mathrm{tr}(\overline{\mathbf{D}}^2) + 2\mu(\overline{\mathbf{D}'\cdot\mathbf{D}'}) = 2\mu\,\mathrm{tr}(\overline{\mathbf{D}}^2) + \varepsilon \geqslant 0. \tag{37}$$

It is evident that in Eq. (37) the turbulent dissipation rate $\varepsilon$, which is generated from taking the ensemble average on the internal dissipation $\delta$, manifests itself as a thermodynamic internal variable. To see the fact, let us consider a simple case – homogeneous turbulent flows, e.g., in decay of homogeneous turbulence (cf. Corrsin, 1963), wherein the gradient of the mean velocity field

$$\mathrm{grad}\,\overline{\mathbf{v}} = \mathbf{0}. \tag{38}$$

Then from Eq. (37), it follows immediately that

$$\overline{\delta} = \varepsilon \geqslant 0, \tag{39}$$

which is directly derived from the Clausius–Planck inequality.

It is worth noting that here as seen, $\varepsilon \geqslant 0$ is a direct consequence of the principle of entropy growth expressed in the form of the Clausius–Planck inequality, without appeal to the *kinematical property* of the turbulent dissipation rate, which reads $\varepsilon \geqslant 0$ as well by definition. That is, the turbulent dissipation rate $\varepsilon$ in itself is a thermodynamic internal variable.

From the turbulent kinetic energy equation, it is evident that in modelling turbulence the thermodynamic internal variable $\varepsilon$ depends on all other unknown terms in the turbulent kinetic equation, meanwhile it has to satisfy its own evolution equation. Therefore, in fact, inequality (37) is not automatically satisfied by an arbitrary closure model employed, but unless on which appropriate restrictions were given, noticing that the turbulent kinetic energy Eq. (35) is not closed. From Eqs. (35) and (37), follows the following inequality that ensures *non-negativeness* of the *mean internal dissipation* $\overline{\delta}$

$$\begin{aligned}&2\mu\,\mathrm{tr}(\overline{\mathbf{D}}^2) - \boldsymbol{\tau}\cdot\overline{\mathbf{D}} + \varrho\overline{\mathbf{b}'\cdot\mathbf{v}'} - \mathrm{div}\left(\overline{p'\mathbf{v}'} + \frac{1}{2}\varrho\overline{(\mathbf{v}'\cdot\mathbf{v}')\mathbf{v}'} - 2\mu\overline{\mathbf{D}'\mathbf{v}'}\right) \\ &\quad = 2\mu\,\mathrm{tr}(\overline{\mathbf{D}}^2) - \boldsymbol{\tau}\cdot\overline{\mathbf{D}} + \varrho\overline{\mathbf{b}'\cdot\mathbf{v}'} - \mathrm{div}\left(\overline{p'\mathbf{v}'} + \frac{1}{2}\varrho\overline{(\mathbf{v}'\cdot\mathbf{v}')\mathbf{v}'}\right. \\ &\quad\quad \left.- \mu\overline{(\mathrm{grad}\,\mathbf{v}' + (\mathrm{grad}\,\mathbf{v}')^{\mathrm{T}})\mathbf{v}'}\right) \\ &\quad \geqslant \mathring{K} = \frac{\partial K}{\partial t} + (\mathrm{grad}\,K)\cdot\overline{\mathbf{v}}. \end{aligned} \tag{40}$$

Setting $\mathbf{b}' = \mathbf{0}$, namely, assuming there is no fluctuation of the body force density, e.g., when $\mathbf{b} = \mathbf{g}$, where $\mathbf{g}$ is the acceleration of gravity prescribed, it follows from Eq. (40) that

$$\begin{aligned}&2\mu\,\mathrm{tr}(\overline{\mathbf{D}}^2) - \boldsymbol{\tau}\cdot\overline{\mathbf{D}} - \mathrm{div}\left(\overline{p'\mathbf{v}'} + \frac{1}{2}\varrho\overline{(\mathbf{v}'\cdot\mathbf{v}')\mathbf{v}'} - 2\mu\overline{\mathbf{D}'\mathbf{v}'}\right) \\ &\quad = 2\mu\,\mathrm{tr}(\overline{\mathbf{D}}^2) - \boldsymbol{\tau}\cdot\overline{\mathbf{D}} - \mathrm{div}\left(\overline{p'\mathbf{v}'} + \frac{1}{2}\varrho\overline{(\mathbf{v}'\cdot\mathbf{v}')\mathbf{v}'}\right. \\ &\quad\quad \left.- \mu\overline{(\mathrm{grad}\,\mathbf{v}' + (\mathrm{grad}\,\mathbf{v}')^{\mathrm{T}})\mathbf{v}'}\right) \\ &\quad \geqslant \mathring{K} = \frac{\partial K}{\partial t} + (\mathrm{grad}\,K)\cdot\overline{\mathbf{v}}. \end{aligned} \tag{41}$$

**Remark 1.** Inequality (41) is a *weak* restriction upon turbulence modelling, which in fact marks the lower bound for the turbulent dissipation rate for any closure model proposed, i.e., $\varepsilon \geqslant -2\mu\,\mathrm{tr}(\overline{\mathbf{D}}^2)$, to be thermodynamically admissible. This constraint indicates that an inappropriate modelling of the Reynolds stress and other unknown correlation terms may lead to a *negative* mean internal dissipation $\overline{\delta}$ and thus becomes incompatible with the principle of entropy growth. It was noted in Sadiki et al. (2000) that some quadratic algebraic stress models tend to produce results like *negative* turbulent kinetic energy. Consequently, this may lead to a negative turbulence dissipation rate so that the mean internal dissipation $\overline{\delta} < 0$.

It is clear that in view of inequality (37) a sufficient condition for non-negativeness of the mean internal dissipation is

$$\varepsilon \geqslant 0. \tag{42}$$

Thus, by Eq. (35) and assuming $\mathbf{b}' = \mathbf{0}$, it follows a *strong* thermodynamic constraint on turbulence modelling,

$$\begin{aligned} &-\boldsymbol{\tau}\cdot\overline{\mathbf{D}} - \operatorname{div}\left(\overline{p'\mathbf{v}'} + \frac{1}{2}\overline{\varrho(\mathbf{v}'\cdot\mathbf{v}')\mathbf{v}'} - 2\mu\overline{\mathbf{D}'\mathbf{v}'}\right) \\ &\quad = -\boldsymbol{\tau}\cdot\overline{\mathbf{D}} - \operatorname{div}\left(\overline{p'\mathbf{v}'} + \frac{1}{2}\overline{\varrho(\mathbf{v}'\cdot\mathbf{v}')\mathbf{v}'} - \mu\overline{(\operatorname{grad}\mathbf{v}' + (\operatorname{grad}\mathbf{v}')^{\mathrm{T}})\mathbf{v}'}\right) \\ &\qquad \geqslant \overset{\circ}{K} = \frac{\partial K}{\partial t} + (\operatorname{grad} K)\cdot\overline{\mathbf{v}}. \end{aligned} \tag{43}$$

**Remark 2.** Eq. (37) implies that in general, in turbulent flows, if at time $t$ and at a point $\mathbf{x}$ where $\operatorname{grad}\overline{\mathbf{v}} = \mathbf{0}$, or at which $\overline{\mathbf{D}} = \mathbf{0}$ while $\overline{\mathbf{W}} = \frac{1}{2}(\operatorname{grad}\overline{\mathbf{v}} + (\operatorname{grad}\overline{\mathbf{v}})^{\mathrm{T}}) \neq \mathbf{0}$, namely, the mean flow is in rigid rotation at $\mathbf{x}$, then the weak restriction (41) coincides with the strong restriction (43). Inequality (43) is a stronger thermodynamic restriction for turbulence modelling than (41), since now the lower bound for the turbulent dissipation rate is zero, i.e., $\varepsilon \geqslant 0$.

Now, let us take a simple example to see the corresponding thermodynamic constraint imposed on the Reynolds stress – homogeneous turbulent shear flow, where

$$(\operatorname{grad}\overline{\mathbf{v}}) = S\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{44}$$

In this case, Eq. (43) gives the following thermodynamic restriction:

$$-S\tau_{12} \geqslant \frac{\partial K}{\partial t}. \tag{45}$$

Note that $K = \frac{1}{2}\tau_{nn}$.

The above inequality implies if it were violated by a closure model for the Reynolds stress, not only would the turbulent dissipation rate $\varepsilon$ become *negative* but also as a result this may lead to a *negative* mean internal dissipation $\overline{\delta}$, if beyond the lower bound for $\varepsilon$, namely, $-2\mu\operatorname{tr}(\overline{\mathbf{D}}^2)$.

For simplicity, consider a linear $K$–$\varepsilon$ model, which reads

$$\boldsymbol{\tau} = \frac{2K}{3}\mathbf{1} + \beta\frac{K^2}{\varepsilon}\overline{\mathbf{D}}, \tag{46}$$

where $\beta$ is a coefficient to be identified.

From Eqs. (44)–(46), we find that

$$-\beta\frac{K^2}{2\varepsilon}S^2 \geqslant \frac{\partial K}{\partial t}. \tag{47}$$

From inequality (47), it follows that $\beta$ cannot be positive, since otherwise $(\partial K/\partial t) \leqslant 0$, but this is impossible because in homogeneous turbulent shear flow the turbulent kinetic energy increases with time (cf. e.g., Speziale, 1991) and actually, as pointed out by Lumley (1970) in this case $K^2/\varepsilon$ is monotonically increasing with time. Thus, the thermodynamic constraint (45) restricts the coefficient $\beta$ within the negative real numbers. In practice, this coefficient takes the value $\beta = -2C_\mu$, where $C_\mu = 0.09$, in the so-called standard $K$–$\varepsilon$ model (cf. Launder and Spalding, 1974), which therefore is consistent with the principle of entropy growth in modelling homogeneous turbulent shear flow.

However, it is important to note that by satisfying the inequality induced by the principle of entropy growth, one can only conclude that the model employed is consistent with the second law of thermodynamics in predicting the given turbulent flow, but this does not imply that the model will do a good job as well in modelling other turbulent flows. In fact, no linear eddy viscosity model can predict secondary flow in a fully developed turbulent flow in a straight tube of non-circular cross-section, because that would require non-zero normal Reynolds stress differences on the cross-section of the tube (cf. Speziale, 1982, 1991; Huang and Rajagopal, 1995).

Let us have a look at another example, a recent model of Yoshizawa and Nisizima (1993), which was developed to capture the so-called non-equilibrium effects of turbulence based on a two-scale direct interaction approximation approach (Kraichnan, 1964). The model of Yoshizawa and Nisizima (1993) takes the form

$$\boldsymbol{\tau} = \frac{2K}{3}\mathbf{1} - \left\{2\nu_t\Big/\left(1 + C_{G1}\frac{K}{\varepsilon}\frac{\mathrm{D}}{\mathrm{D}t}\log\nu_t\right)\right\}\overline{\mathbf{D}}, \tag{48}$$

where $\nu_t = C_\mu(K^2/\varepsilon)$, $C_\mu = 0.09$, and $C_{G1}$ is to be identified.

An approximation form of model (48) of Yoshizawa and Nisizima (1993) reads

$$\boldsymbol{\tau} = \frac{2K}{3}\mathbf{1} - 2C_\mu\frac{K^2}{\varepsilon}\overline{\mathbf{D}} - 2C_{G1}C_\mu\frac{K^2}{\varepsilon^3}(K\dot{\varepsilon} - 2\dot{K}\varepsilon)\overline{\mathbf{D}}. \tag{49}$$

Substituting Eqs. (48) and (44) into inequality (45), we obtain

$$\begin{aligned} &\nu_t S^2\Big/\left(1 + C_{G1}\frac{K}{\varepsilon}\frac{\mathrm{D}}{\mathrm{D}t}\log\nu_t\right) \\ &\quad = C_\mu\frac{K^2}{\varepsilon}S^2\Big/\left(1 + C_{G1}\frac{K}{\varepsilon}\frac{\mathrm{D}}{\mathrm{D}t}\log\left(C_\mu\frac{K^2}{\varepsilon}\right)\right) \geqslant \frac{\partial K}{\partial t}. \end{aligned} \tag{50}$$

Now, recalling that $K^2/\varepsilon$ increases monotonically with time and noting that $\varepsilon \leqslant SK$, it is evident that inequality (50) confines the coefficient $C_{G1}$ to be a positive number, since otherwise, during the shearing process it would happen that $(\partial K/\partial t) \leqslant 0$, but this is impossible. In the model of Yoshizawa and Nisizima (1993), the coefficient $C_{G1}$ was indentified as $C_{G1} = 1.3$, with recourse to the DNS data. Again, we see that the model coefficient $C_{G1}$ is confined to be such that the modelling is compatible with the second law of thermodynamics. Of course, it is not impossible that this coefficient $C_{G1}$ could be identified as a *negative* number if the DNS date were flawed. Nonetheless, the thermodynamic constraint as seen demarks clearly the region to which $C_{G1}$ should belong.

In closing, we have shown that the principle of entropy growth, expressed in terms of the Clausius–Duhem and the Clausius–Planck inequalities, imposes restrictions upon turbulence modelling, wherein the turbulent dissipation rate $\varepsilon$, as a thermodynamic internal variable, plays a key role in ensuring non-negativeness of the mean internal dissipation $\overline{\delta}$ such that the modelling is thermodynamically admissible.


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