

On Thermodynamic Consistency of Turbulent Closures*

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Abstract. The problem of the implementation of the second law of thermodynamics for the determination of the thermodynamic consistency of solutions determined by turbulent closures is considered for incompressible fluids. The possibility of the application of the methods of thermodynamics to constraining constitutive laws describing turbulent flow features, but not material behaviour, is discussed. It is shown that the ordinary realizability conditions requiring non-negative values of the averaged squared fluctuations are necessary and sufficient conditions determining the thermodynamic consistency of a process governed by a closure model. Because turbulent closures are not universal, using the second law of thermodynamics to constrain them can impose unnecessary restrictions on the models, when the turbulent entropy is considered as a constitutive quantity. The notion and validity of different forms of the turbulent entropy is discussed. It is found that the form of the turbulent entropy originating from the analogy between the turbulent kinetic energy and absolute temperature contradicts the principle of irreversibility. In a particular case of small temperature fluctuations, the second law yields correct constraints, if the turbulent entropy is assumed not to be a constitutive quantity, but a variable governed by an evolution equation of special form generated by the balance equation for internal energy.

1. Introduction

Turbulence is present almost everywhere in geophysical and engineering flows. It manifests itself as a chaotic form of the motion due to instabilities that arise at sufficiently high Reynolds numbers. In fluid dynamics this highly violent motion can be described by the Navier–Stokes–Fourier equations provided the small-scale processes are resolved in the numerical integration procedures for these field equations (Reynolds, 1990). Alternatively, turbulent flow is governed by balance equations that describe the average characteristics of the persistent flow structure. Therefore, eddy-viscosity-based models (Boussinesq, 1877) and Reynolds-stress models (Rotta, 1951) use ensemble averaging of the fields in space and time. Common to all different modelling approaches is that they lead to non-closed systems of equations for the mean fields and correlation terms. The derivation of equations for higher-order correlations does not lead to a system in closed form. Therefore, the problem of closing the system of averaged balance equations arises; its performance is reminiscent of the postulation of constitutive relations in continuum thermodynamics.

Any closure model developed to be as universal as possible is supposed to satisfy what is called in turbulence modelling the “realizability conditions” determining the physical consistency of the derived solution

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(Schumann, 1977; Lumley, 1978). Moreover, it must be consistent with the second law of thermodynamics, because every possible process of a system is characterized by non-negative entropy production. This can impose constraints on the closing functional dependencies or on constitutive parameters, when the form of the functional dependencies is assumed in an *ad hoc* fashion. It is a condition of continuum thermodynamics that constitutive laws describing material behaviour must guarantee satisfaction of the second law of thermodynamics for any thermodynamic process of a system (Coleman and Noll, 1963). In this case it is usually possible to find such constraints from the entropy principle. This approach to study the thermodynamic consistency of turbulent one-point algebraic closures has been applied by Ahmadi (1985, 1988, 1989). However, one of the weakest points in such an analysis is the assumption of the constitutive law for the entropy. Usually it is based on the similarity of the chaotic turbulent motion of the particles and the chaotic motion of the molecules, which suggests assuming that the turbulent kinetic energy can be considered as the second temperature determining the corresponding “turbulent entropy” (Ahmadi, 1985; Marshall and Naghdi, 1989). This assumption can be questioned, because, while there is significant difference between the scales of molecular and macroscopic motions, there is no significant difference between the scales of the mean and turbulent motions. Moreover, the physics of molecular and turbulent motions is different.

Thermodynamics of continua implies the existence of universal constitutive laws valid for a sufficiently wide range of flows. Therefore another problem that arises in the application of the methods of thermodynamics is caused by the assumption that all types of turbulent flows can be described by a closure for the Reynolds-averaged Navier–Stokes–Fourier equations with local-type closing functional dependencies. Although some types of flow can be described within the framework of this approach, this is generally not correct for existing one-point turbulent closures because of the importance of non-local interactions, in particular, determined by pressure fluctuations (e.g. Bradshaw, 1976). Hence, application of the local entropy principle requiring satisfaction of the second law for any solution determined by a model can impose unnecessary constraints on it.

The problems discussed above can question the possibility of the implementation of irreversible thermodynamics to turbulence modelling in general. In particular, Speziale (1999) insists on the inapplicability of the second law for the mean fields. However, Rajagopal (1999) questions Speziale’s claim as Speziale points to no internal inconsistencies, nor does he offer any physical explanation for not appealing to some form of the entropy inequality. Rajagopal (1999) also points to Speziale’s reason as being a mere belief as Speziale states “there is no reason to *believe* it (the Clausius–Duhem inequality) is necessarily satisfied by the Reynolds averaged fields ...”. Such controversy shows that the problem is not yet completely understood and requires further investigation.

In this work, in order to find thermodynamical constraints, we base our analysis on the second law of thermodynamics written in non-averaged variables, which is similar to the analysis performed by Speziale (1999). In Section 2 we search for the conditions guaranteeing that a thermodynamic process satisfying them will be consistent with the second law of thermodynamics. Application of methods of thermodynamics to developing thermodynamically consistent closures and the notion of the turbulent entropy are discussed in Section 3. We consider the flow of only the volume-preserving Navier–Stokes–Fourier fluid.

2. Analysis

2.1. Governing Equations

In what follows Cartesian tensor notation is employed with the Einstein summation convention over doubly repeated indices. If t_{ij} is a second rank tensor, then $t_{(ij)}$ will denote its traceless, deviatoric part. Non-averaged fields will carry a tilde, mean values (except the turbulent kinetic energy k and its dissipation rate ε) will be denoted by capital letters, and the fluctuation of a field quantity from its mean value will be denoted by lower-case letters: e.g. $\tilde{\theta} = \Theta + \theta$. Bars will identify ensemble averaging. Scales will be identified by brackets. The symbol O means an order of magnitude.

The following notations are used: \tilde{u}_i is the velocity vector, τ is the time, \tilde{t}_{ij} is the stress tensor, $\tilde{d}_{(ij)}$ is the strain-rate deviator tensor, \tilde{q}_i is the heat flux vector, $\tilde{\theta}$ is the absolute temperature, $C_v = \text{const}$ is the heat capacity, $\tilde{e} = C_v \tilde{\theta}$ is the specific internal energy, \tilde{p} is the pressure, \tilde{s} is the specific entropy, $\tilde{\phi}_i$ is the non-convective entropy flux, k is the specific turbulent kinetic energy, ε is the specific turbulent dissipation rate,

and $\rho = \text{const}$ is the density; μ and ν are the dynamic and kinematic viscosities, λ is the heat conductivity, ρR_{ij} is the Reynolds stress tensor, and \tilde{f}_i is the body force vector. We assume that the heat capacity is constant, and that the temperature fluctuations influence the viscosities and heat conductivity negligibly (Bradshaw, 1976).

The balance laws of mass, linear momentum and internal energy, referred to an inertial frame, are

$$\tilde{u}_{i,i} = 0, \quad (1)$$

$$\dot{\tilde{u}}_i = \frac{1}{\rho} \tilde{t}_{ij,j} + \tilde{f}_i, \quad (2)$$

$$\rho \dot{\tilde{e}} + \tilde{q}_{i,i} = \tilde{t}_{(ij)} \tilde{u}_{i,j}, \quad (3)$$

and the second law of thermodynamics takes the form

$$\rho \dot{\tilde{s}} + \tilde{\phi}_{i,i} \geq 0, \quad (4)$$

an inequality requiring entropy production to be positive for all thermodynamic processes. In the above

$$\dot{\tilde{y}} := \frac{\partial \tilde{y}}{\partial \tau} + \tilde{u}_i \tilde{y}_{,i} \quad (5)$$

is the total or material time derivative.

The above balance equations must be supplemented by constitutive equations for the internal energy \tilde{e} , stresses \tilde{t}_{ij} and heat fluxes \tilde{q}_i . The internal energy is assumed to be linearly dependent on the absolute temperature. Constitutive laws for a Navier–Stokes–Fourier fluid imply the following quasi-linear constitutive relations:

$$\tilde{e} = C_v \tilde{\theta}, \quad \tilde{t}_{ij} = -p \delta_{ij} + 2\mu(\tilde{\theta}) \tilde{d}_{(ij)}, \quad \tilde{q}_i = -\lambda(\tilde{\theta}) \tilde{\theta}_{,i}. \quad (6)$$

Application of the methods of irreversible thermodynamics leads to exactly these relations, and the conditions $\mu \geq 0$, $\lambda \geq 0$ guarantee satisfaction of the entropy inequality. These constitutive relations proved to describe a wide range of thermodynamic processes, however, the equations suffer from the disadvantage of an infinite rate of propagation of thermomechanical disturbances, and model thermodynamic processes with high frequencies of fluctuations inadequately (Müller and Ruggeri, 1993; Jou *et al.*, 1996), which may also be the case in turbulent flows. On the other hand, Stewart (1951) verified experimentally the von Kármán–Howarth dynamic equation for isotropic turbulence, which is derived from the Navier–Stokes equations. Moreover, while the relaxation time for fluids is found to be of the order of 10^{-12} s, the period of turbulent fluctuations in flows under consideration reaches only 10^{-5} – 10^{-6} s (Moulden *et al.*, 1977). This is a reason for us to conjecture sufficient validity of the Navier–Stokes–Fourier equations at all practical length and time scales of the eddies. This means that the turbulent flow as a thermodynamic process is assumed to be satisfactorily described by the velocities, strain-rates, temperature and temperature gradient as the only independent variables, and the entropy constitutive law can be satisfactorily approximated by its version assumed by irreversible thermodynamics of simple fluids $\tilde{s} = C_v \ln \tilde{\theta}$. Therefore, the second law of thermodynamics can be written in Clausius–Duhem form:

$$\rho \dot{\tilde{s}} + \frac{\partial}{\partial x_i} \left(\frac{\tilde{q}_i}{\tilde{\theta}} \right) \geq 0, \quad \tilde{s} = C_v \ln \tilde{\theta}. \quad (7)$$

Because $\dot{\tilde{s}} = C_v \dot{\tilde{\theta}}/\tilde{\theta}$, after eliminating $\dot{\tilde{s}}$ with the help of (3) and (6)₁, one can derive the necessary and sufficient condition of thermodynamic consistency of a process in the form

$$-\frac{1}{\tilde{\theta}^2} \tilde{q}_i \tilde{\theta}_{,i} + \frac{1}{\tilde{\theta}} \tilde{t}_{(ij)} \tilde{d}_{(ij)} \geq 0. \quad (8)$$

Since $\tilde{\theta} > 0$ we can rewrite this inequality in the sufficient form via the two inequalities

$$-\tilde{q}_i \tilde{\theta}_{,i} \geq 0, \quad \tilde{t}_{(ij)} \tilde{d}_{(ij)} \geq 0. \quad (9)$$

2.2. Averaged Governing Equations

Assuming negligible influence of the temperature fluctuations on the viscosity and heat conductivity (Bradshaw, 1976), after decomposition of the fields into the mean and fluctuating parts, we can write the averaged balance equations as (the entropy inequality will be treated later)

$$U_{i,i} = 0, \quad (10)$$

$$U_i^\bullet = \frac{1}{\rho} T_{ij,j} + R_{ij,j} + F_i, \quad (11)$$

$$\rho E^\bullet = -Q_{i,i} - \rho Q_{i,i}^T + T_{(ij)} U_{i,j} + \rho \varepsilon, \quad (12)$$

where

$$Y^\bullet = \frac{\partial Y}{\partial \tau} + U_i Y_{,i} \quad (13)$$

and

$$\begin{aligned} R_{ij} &= -\overline{u_i u_j}, & Q_i^T &= \overline{e u_i}, & k &= \frac{1}{2} R_{ii}, \\ T_{ij} &= -P + 2\mu D_{(ij)}, & Q_i &= -\lambda \Theta_{,i}, & \varepsilon &= 2\nu d_{(i,j)} d_{(i,j)} \approx \nu \overline{u_{i,j} u_{i,j}}. \end{aligned} \quad (14)$$

The conditions $k \geq 0$, $\varepsilon \geq 0$ are evident conditions of realizability (Schumann, 1977), which must hold by definition. k and ε are called the turbulent kinetic energy and its dissipation rate.

2.3. Implementation of the Second Law

The system of equations (10)–(14) is not closed because $R_{(ij)}$, Q_i^T , ε and k are not known. In modelling turbulent flows these parameters are assumed to depend on the mean quantities through the corresponding constitutive relations, or corresponding balance equations for them are used with closing relations for the higher-order turbulent correlations. For example, a standard k – ε model assumes

$$R_{(ij)} = 2\nu_T D_{(ij)}, \quad \nu_T = C_\mu \frac{k^2}{\varepsilon}, \quad Q_i^T = -\frac{\nu_T}{\zeta_e} \Theta_{,i}, \quad (15)$$

$$k^\bullet = 2\nu_T D_{(ij)} D_{(ij)} + \frac{\partial}{\partial x_i} \left[\left(\nu + \frac{\nu_T}{\zeta_k} \right) k_{,i} \right] - \varepsilon, \quad (16)$$

$$\varepsilon^\bullet = C_{\varepsilon 1} \frac{\varepsilon}{k} 2\nu_T D_{(ij)} D_{(ij)} + \frac{\partial}{\partial x_i} \left[\left(\nu + \frac{\nu_T}{\zeta_\varepsilon} \right) \varepsilon_{,i} \right] - C_{\varepsilon 2} \frac{\varepsilon^2}{k}, \quad (17)$$

where C_μ , $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, ζ_e , ζ_k , ζ_ε are constants. In either way, a sought solution must satisfy the second law. The inequalities (9) are satisfied for the non-averaged values due to the constitutive laws of Fourier and Navier–Stokes with non-negative viscosity and heat conductivity. However, because turbulent models operate with the mean values and correlations, we must find corresponding constraints for them. Averaging the sufficient conditions (9) yields

$$\Theta_{,i} \Theta_{,i} + \overline{\theta_{,i} \theta_{,i}} \geq 0, \quad \mu D_{(ij)} D_{(ij)} + \rho \varepsilon \geq 0. \quad (18)$$

Both inequalities are obviously satisfied: the terms on the left-hand sides are all non-negative by mere definition of the quantities involved. This is so despite the fact that in many closure models the term $\overline{\theta_{,i} \theta_{,i}}$ is not modelled because it does not enter the balance equations. Moreover, the parameter $\overline{\theta_{,i} \theta_{,i}}$ can be considered a non-negative constitutive quantity, and this will not change the solution and the conclusion of thermodynamic consistency regardless of the specific constitutive law for it. Alternatively, if $\overline{\theta_{,i} \theta_{,i}}$ is modelled in a closure scheme, then the condition $\overline{\theta_{,i} \theta_{,i}} \geq 0$ must be satisfied as a realizability condition. The same is true for ε , since it is non-negative by definition. Therefore, the realizability conditions are sufficient conditions of thermodynamic consistency of a solution determined by a closure.

On the other hand, any thermodynamically consistent process which the *physical system*¹ may undergo satisfies the realizability conditions, otherwise such a process is impossible. Hence, the realizability conditions are necessary and sufficient conditions of thermodynamic consistency of a solution described by a model.

We conclude that the requirement of thermodynamic consistency of a solution does not impose any additional constraints except the realizability conditions, because by assuming local equilibrium the second law insists only on the irreversible conversion of the kinetic energy of motion into internal heat and molecular (not turbulent) heat flow in the direction opposite to the temperature gradients. This is satisfied by assuming non-negative values of the thermal conductivity and dynamic viscosity, while the closure models for R_{ij} and Q_j^T are approximations of the convective fluxes. Again, as was pointed out by Speziale (1999), the system of the non-averaged Navier–Stokes–Fourier equations with non-negative values of the thermal conductivity and dynamic viscosity determines thermodynamic consistency of all the solutions, therefore if a closure for the Reynolds-averaged Navier–Stokes–Fourier equations describes some types of flow correctly, then it determines thermodynamically consistent solutions satisfying the realizability conditions. If a closure does not model some types of flows correctly, then thermodynamic inconsistency determined by non-physical values of some solutions shows inadequacy of the derived results. At the same time, the thermodynamic consistency of a solution described by a closure scheme does not guarantee that it is a correct solution of the Reynolds-averaged Navier–Stokes–Fourier equations.

It should be noted that if the turbulent dissipation rate ε is considered as an independent variable, whose evolution is described by the corresponding balance equation (as it is in the majority of turbulence models), then the requirement² $\varepsilon \geq 0$ is a constraint on the domain of definition of this variable, but not on the constitutive dependencies, as could be expected in the thermodynamics of continua.

Development of turbulent closures satisfying the realizability conditions is out of the scope of this work (for discussion see, e.g. Abid *et al.*, 1994).

3. Constraining Turbulent Closures by Irreversible Thermodynamics

The results presented above were derived by quite simple analysis based only on the assumption of local thermodynamic equilibrium, which determines the validity of the Navier–Stokes–Fourier equations and the Clausius–Duhem inequality for entropy production. We found conditions determining the thermodynamic consistency of a solution described by a one-point model. This analysis, however, does not follow the formal approach of thermodynamics, searching for the constitutive relations of entropy and entropy flux (as well as of the other dependent quantities) in terms of the independent variables adopted by a specific model and guaranteeing that all the solutions determined by a closure scheme will be thermodynamically consistent. Therefore, below we consider this approach of the implementation of the second law to show problems arising in following it when turbulent flow features, but not material behaviour, are modelled, and how these problems can be overcome in some situations. First, we show that the turbulent entropy cannot be neglected in a thermodynamic analysis. Then the inapplicability of one commonly used constitutive law for the turbulent entropy is demonstrated. In Section 3.3 we show that non-universality of the models can lead to unnecessary constraints imposed by the second law. At the end of this section an evolution equation for the turbulent entropy is suggested for a particular class of flows, which yields results consistent with those derived in the previous section.

3.1. Influence of a Small Value of the Turbulent Entropy on the Mean Entropy Change

Treating the entropy inequality (7)₁ we first eliminated the material derivative of the entropy $\dot{\bar{s}}$ with the help of the entropy constitutive law (7)₂ and the energy equation (3) and only then performed the averaging process. Alternatively, towards implementation of the methods of thermodynamics, averaging of (4) and (7)₂ is

¹ We specially point out that we consider processes permitted by the physical system, because considering solutions not describing physical processes to find the necessary conditions of thermodynamical consistency is not required. Therefore, we also speak about the thermodynamical consistency of a solution, but not of the model.

² Evidently, an arbitrary form of the evolution equation for ε can generally determine a negative value of ε .

performed instead; it yields

$$S = C_v \ln \Theta + S^T, \quad (19)$$

$$\rho S^\bullet + \Phi_{i,i} \geq 0, \quad (20)$$

where

$$\Phi_i = \rho \overline{u_i s} - \frac{\lambda \overline{\tilde{\theta}_{,i}}}{\overline{\tilde{\theta}}}, \quad (21)$$

$$S^T = C_v \overline{\ln(\Theta + \theta)} - C_v \ln \Theta. \quad (22)$$

S^T is usually called the turbulent entropy, and Φ_i is the mean-cumulative entropy flux including the molecular and turbulent entropy transfer. It should be noted that the definitions of Φ_i and S^T are direct consequences of the Clausius–Duhem inequality and the constitutive law for the entropy (7).

If the typical temperature difference in the system $[\Delta\Theta]$ is much smaller than the absolute temperature, $[\Delta\Theta] \ll [\Theta]$, and the temperature fluctuations are comparable with it, $\theta \sim [\Delta\Theta]$, which is characteristic for most turbulent flows, then using expansions in terms of $\theta/\Theta \ll 1$ we obtain

$$S^T = -C_v \frac{\overline{\theta^2}}{2\Theta^2} + O\left(C_v \frac{\overline{\theta^3}}{\Theta^3}\right) \leq 0, \quad (23)$$

$$\overline{u_i s} = \frac{Q_i^T}{\Theta} - C_v \frac{\overline{u_i \theta^2}}{2\Theta^2} + O\left(C_v \frac{\overline{u_i \theta^3}}{\Theta^3}\right), \quad (24)$$

$$\left(\frac{\overline{\tilde{\theta}_{,i}}}{\overline{\tilde{\theta}}}\right) = \frac{\overline{\theta_{,i}}}{\Theta} - \frac{\overline{\theta_{,i}\theta}}{\Theta^2} + O\left(\frac{\overline{\theta_{,i}\theta^2}}{\Theta^3}\right). \quad (25)$$

As the lowest-order algebraic dependency we assume $Q_i^T = -\gamma \Theta_{,i}/\rho$, where γ depends on ε and k . Then, after neglecting the higher-order terms in (23)–(25), due to (12), (23)–(25) the entropy inequality (20) takes the form

$$\frac{\lambda + \gamma}{\Theta^2} \Theta_{,i} \Theta_{,i} - \rho C_v \frac{\overline{\frac{1}{2}\theta^2}}{\Theta^2} + \frac{1}{\Theta} (\mu D_{(ij)} D_{(ij)} + \rho \varepsilon) + \hat{\Phi}_{i,i} \geq 0, \quad (26)$$

where

$$\hat{\Phi}_i := \frac{\lambda}{\Theta^2} \frac{\partial \overline{\frac{1}{2}\theta^2}}{\partial x_i} - \rho C_v \frac{\overline{u_i \frac{1}{2}\theta^2}}{\Theta^2} = \Phi_i - \frac{\rho Q_i^T}{\Theta} + \lambda \frac{\Theta_{,i}}{\Theta} \quad (27)$$

is the excess entropy flux. In deriving (26) we also neglected $\overline{\theta^2} \Theta^\bullet / \Theta^3 \sim [\Delta\Theta]^3 / [\tau][\Theta]^3$ in comparison with $\overline{\theta^2} / \Theta^2 \sim [\Delta\Theta]^2 / [\tau][\Theta]^2$, where $[\tau]$ is the characteristic time scale of the mean flow. From (19) we obtain $S^\bullet = C_v \Theta^\bullet / \Theta + S^{T^\bullet}$, where the ratio of the second term (change of the turbulent entropy) to the first one (change of the mean-field entropy) on the right-hand side can be estimated as $[\Delta\Theta]/[\Theta] \ll 1$. At the same time, the energy equation (12) yields, in terms of scales, $\rho C_v [\Delta\Theta]/[\tau] = [\lambda + \gamma][\Delta\Theta]/[x]^2$, where $[x]$ is the spatial scale of the mean flow, hence we conclude that the first two terms in (26), estimated as $[\lambda + \gamma][\Delta\Theta]^2/[\Theta]^2[x]^2$ and $\rho C_v [\Delta\Theta]^2/[\Theta]^2[\tau]$, respectively, are of the same order. Therefore, we cannot neglect the second term in (26), representing the change of the turbulent entropy S^T , to study thermodynamic consistency. This means that the turbulent entropy is an important characteristic which must be treated, although it is small in the case under consideration. Fortunately, we avoided this problem by performing the averaging after elimination of the entropy in the entropy inequality. A similar analysis shows that neither we can neglect the second terms on the right-hand sides of (24)–(25), although they are small in comparison with the first terms. In particular, this means that when the turbulent entropy is considered as a constitutive quantity, then the mean-cumulative entropy flux Φ_i cannot be presented in the simple diffusive form $\Phi_i = (\lambda + \gamma)\Theta_{,i}/\Theta$, as could be expected in analogy with the molecular entropy flux.

3.2. Turbulent Entropy Determined by Turbulent Temperature

In order to apply the methods of thermodynamics, the constitutive law for the turbulent entropy S^T must be determined. One of the broadly used assumptions to determine it is to regard the turbulent kinetic energy as a “turbulent temperature”, on the basis of the analogy between the chaotic molecular motion and the chaotic turbulent motion of fluid particles. One then considers a turbulent flow as a flow of a multi-component fluid (e.g. Ahmadi, 1985, 1988, 1989; Marshall and Naghdi, 1989). Such an approach seems quite attractive – to obtain restrictions on possible models of redistribution or transfer of the turbulent kinetic energy based on the concept of irreversibility. However, the processes are definitely macroscopic and governed by the Navier–Stokes–Fourier equations, while the second law assuming local thermodynamic equilibrium (which can be adopted in modelling turbulence) insists on irreversibility associated only with energy dissipation and heat flux in opposition to the temperature gradient. Moreover, from (22) it is clear that the turbulent entropy is determined only by the temperature fluctuations. Furthermore, if at some instant or some place there are statistically no fluctuations of temperature, then the turbulent entropy is equal to zero regardless of the value of the turbulent kinetic energy. It is also known (e.g. Hallböck *et al.*, 1995) that the turbulent kinetic energy production can be temporally and locally negative under some conditions. This means that the “turbulent temperature” can be converted into energy of the mean flow, but this contradicts the notion of irreversibility associated with the absolute temperature.

On the other hand, inadequacy of the assumption that the turbulent kinetic energy is equivalent to the temperature in defining the turbulent entropy can be shown by investigating the entropy constitutive law found by Ahmadi (1989) on the basis of the theory of multi-temperature fluids (Ahmadi, 1985):

$$S = C_v \ln \Theta + S^T, \quad S^T = C_0^T \varepsilon (\ln k - \alpha \ln \varepsilon - C_0).$$

Here, $C_0^T > 0$, $\alpha > 0$, C_0 are constants. In order to ascertain the validity of this equation we consider the case of decaying isotropic turbulence in a closed system in the absence of a mean flow. We can impose the initial values of k , ε and Θ , denoted by subscript 0, as arbitrary positive constants.³ In particular, $C_0^T \varepsilon_0 = m C_v$, where $m > 1$, is a permissible initial value for ε_0 . Again, it is reasonable to assume that eventually equilibrium will be reached with the corresponding equilibrium entropy $S_E = C_v \ln \Theta_E$, where the equilibrium temperature $\Theta_E = \Theta_0 + k_0/C_v$, because all the turbulent kinetic energy will dissipate into heat, and this will increase the fluid temperature by the corresponding value k_0/C_v . In this case

$$S_E - S_0 = C_v \ln \left(\frac{\Theta_0}{k_0^m} + \frac{1}{[C_v k_0^{m-1}]} \right) + C_0^T \varepsilon_0 (\alpha \ln \varepsilon_0 + C_0) - C_v \ln \Theta_0.$$

Evidently, for sufficiently large k_0 , and in particular as $k_0 \rightarrow \infty$, the right-hand side is negative and so $S_E - S_0 < 0$, hence $S_E < S_0$. Thus, the entropy of the process under consideration decreases, which under adiabatic conditions contradicts the second law of thermodynamics. This conclusion was derived only by investigating the constitutive law for the entropy, therefore the determined thermodynamic inconsistency of the model is only due to the applied constitutive relation for the entropy, but not due to the inadequacy of the closure scheme, whatever the latter may be. This means that considering the turbulent kinetic energy as the turbulent temperature determining turbulent entropy seems to be inadequate.

3.3. Analysis of the Thermodynamic Consistency of the k – ε Model

Thermodynamics of continua assumes that adopted constitutive relations can describe material behaviour for a sufficiently wide range of processes. The form of these relations and values of constitutive parameters entering them are fixed for a particular material. The Navier–Stokes–Fourier equations are adequate for not very large values of $\dot{d}_{(ij)}$ and $\dot{\theta}_{,i}$ (Jou *et al.*, 1996). These variables do not enter the governing equations and are independent, hence, the Navier–Stokes–Fourier equations are valid for any value of the independent fields and their independent derivatives entering them. The constitutive relations must guarantee thermodynamic consistency of all possible solutions of the governing equations, which will determine

³ These initial values will determine the coefficient of proportionality in the self-similar decay $k \propto \varepsilon^\alpha$.

constraints on the constitutive parameters. Material behaviour cannot be described by constitutive laws not satisfying these constraints because of the universal nature of these laws. For example, formally there exist thermodynamically consistent solutions of the Navier–Stokes–Fourier equations with a negative value of the molecular viscosity, if we consider large temperature gradients and small strain-rates. At the same time, it is possible to find an inconsistent solution with such a negative value of the viscosity in considering small values of temperature gradients, or high strain-rates. This means that such a process cannot be described by the adopted constitutive law with negative viscosity, and this contradicts the assumption of universality of the model. Therefore, a universal model can exist only when the value of the viscosity is non-negative.

Such an approach is quite effective in modelling material behaviour, however, it may not be justified in modelling turbulence because a universal model describing all types of turbulent flows does not exist yet. Every particular model is able to describe only a limited range of flows. Moreover, values of the parameters entering the closing relations of a model can be different for different types of flows that can be described by the closure. Therefore, the conclusion that some particular value of a constitutive parameter determines an inconsistent solution can be made in considering a process which cannot be described in the context of the applied model, while some other processes can be described by the model using the very value of the parameter. Only the latter processes must be considered in order to find necessary constraints on the constitutive parameters. However, how to perform this procedure is not yet clear. Hence, the requirement of thermodynamic consistency of all the solutions determined by a model can impose unnecessary constraints on the model, because such constraints can be found in considering processes beyond the validity of the employed form of the constitutive laws. In particular, this can be shown in analysing the standard k – ε model (Jones and Launder, 1972) as follows.

In applications of thermodynamics to the k – ε model in a general way, one assumes that the turbulent entropy depends on all the independent fields adopted by the closure and physical parameters entering the Reynolds-averaged Navier–Stokes–Fourier equations. In this case we can write⁴ $S^T = S^T(\Theta, D_{(ij)}, \Theta_{,i}, k, \varepsilon)$, $\Phi_i = \Phi_i(\Theta, D_{(ij)}, \Theta_{,i}, k, \varepsilon)$. The entropy inequality takes the form

$$C_v \frac{\Theta^\bullet}{\Theta} + \frac{\partial S^T}{\partial \Theta} \Theta^\bullet + \frac{\partial S^T}{\partial D_{(ij)}} D_{(ij)}^\bullet + \frac{\partial S^T}{\partial \Theta_{,i}} \Theta_{,i}^\bullet + \frac{\partial S^T}{\partial k} k^\bullet + \frac{\partial S^T}{\partial \varepsilon} \varepsilon^\bullet + \frac{1}{\rho} \Phi_{i,i} \geq 0. \quad (28)$$

Because this inequality is constrained by the balance equations for the independent fields Θ , k , ε , their total derivatives must be eliminated in (28) with the help of the balance equations. The material derivatives $D_{(ij)}^\bullet$ and $\Theta_{,i}^\bullet$ are not constrained by the balance equations and can take any values. As was shown in Section 3.1, the turbulent entropy cannot generally be neglected and is determined only by the temperature fluctuations. In particular, the typical value of the temperature fluctuations is determined by the typical temperature difference in the system $[\Delta\Theta]$, therefore physical considerations imply the necessary dependence of S^T on the mean temperature gradient $\Theta_{,i}$: $\partial S^T / \partial \Theta_{,i} \neq 0$. Because $\Theta_{,i}^\bullet$ does not enter the balance and constitutive relations, the requirement that the second law be satisfied for *any* process in the system will be determined from the entropy principle $\partial S^T / \partial \Theta_{,i} = 0$, guaranteeing $\Theta_{,i}^\bullet \partial S^T / \partial \Theta_{,i} = 0$, $\forall \Theta_{,i}^\bullet$, otherwise there are thermodynamically inconsistent processes. Because generally $\partial S^T / \partial \Theta_{,i} \neq 0$ and, as was shown in Section 3.1, the influence of the turbulent entropy on the mean entropy change is significant, which means that the value of $\Theta_{,i}^\bullet \partial S^T / \partial \Theta_{,i}$ is not negligible, the k – ε model determines thermodynamically inconsistent solutions *regardless of the closing dependencies employed* and therefore is inconsistent. However, the linear model describes simple shear fairly well, and the non-linear model has an even wider range of applicability, in particular, by accounting for effects of rotation and describing non-isothermal flows of a turbulent impinging jet (Craft *et al.*, 1993). Hence, the derived conclusion is not informative for modelling turbulence.

The implied inconsistency of the k – ε model is associated at least with the quantity $\Theta_{,i}^\bullet$ (it can also be associated with the quantity $D_{(ij)}^\bullet$ if the dependence of S^T on $D_{(ij)}$ is not weak). This can be explained by the inadequacy of the eddy-diffusivity-based constitutive relation for the turbulent heat flux $Q_i^T = -\gamma \Theta_{,i} / \rho$ to describe relaxation processes with high values of $\Theta_{,i}^\bullet$. For example, this relation implies the absence of the turbulent heat flux after a sharp fall of the mean heat flux $\Theta_{,i}$ to zero. However, this is not the case for turbulent flows. Therefore, in such situations the turbulent heat flux is poorly approximated by the applied constitutive relation, hence, the obtained solution of the mathematical model will be physically inadequate.

⁴ Possible presence of the vorticity tensor in the constitutive laws does not influence the present analysis.

This means that the conclusion about inconsistency points only to the inability of the employed model to describe some types of processes adequately, which can also be determined by non-physical values, whereas other types of flow can be described correctly.

3.4. Towards a Self-Consistent Analysis

Here we consider only the class of solutions satisfying the condition $[\Delta\Theta]/[\Theta] \ll 1$. First, it should be noted that the conditions of thermodynamic consistency derived in Section 2 were obtained by analysing the second law constrained by the Navier–Stokes–Fourier equations. This means that these conditions for averaged quantities were derived by considering only those solutions determined by a closure which are correct solutions of the Reynolds-averaged Navier–Stokes–Fourier equations. We therefore avoided derivation of unnecessary constraints that could be obtained by considering processes that cannot be described in the context of the closure scheme. In particular, it was concluded that the value of the eddy diffusivity γ is not constrained, whereas, because γ enters the balance equation for the temperature (12) and the entropy inequality (26), we could generally expect that γ must be constrained to ensure a non-negative value of the entropy production. However, if a process can be described by a closure, then considering a higher-order model, which includes equations for higher-order correlations, will determine the same solution with sufficient order of accuracy. In this case we can identically transform the entropy inequality (26), using a balance equation for a higher-order moment. In order to find the value of the total derivative of the turbulent entropy we can use the balance equation for $\overline{\frac{1}{2}\theta^2}$ (Corrsin, 1952):

$$\rho C_v \overline{\frac{1}{2}\theta^2}^\bullet = -\rho Q_i^T \Theta_{,i} + \frac{\partial}{\partial x_i} \left(\Theta^2 \hat{\Phi}_i \right) - \lambda \overline{\theta_{,i}\theta_{,i}} + 2\mu D_{(ij)} \overline{\theta d_{(ij)}} + \mu \overline{\theta d_{(ij)} d_{(ij)}}. \quad (29)$$

Using the expression for the turbulent heat flux $Q_i^T = -\gamma \Theta_{,i} / \rho$, after elimination of $\overline{\frac{1}{2}\theta^2}^\bullet$ in (26) with the aid of (29) we can derive the entropy inequality, which does not include the eddy diffusivity γ :

$$\frac{\lambda}{\Theta^2} \Theta_{,i} \Theta_{,i} + \frac{1}{\Theta} (\mu D_{(ij)} D_{(ij)} + \rho \varepsilon) + \lambda \xi - \frac{2}{\Theta} \Theta_{,i} \hat{\Phi}_i - \frac{1}{\Theta^2} (2\mu D_{(ij)} \overline{\theta d_{(ij)}} + \mu \overline{\theta d_{(ij)}^2}) \geq 0, \quad (30)$$

where $\xi := \overline{\theta_{,i}\theta_{,i}} / \Theta^2 \geq 0$. Therefore, the value of the eddy diffusivity γ cannot be constrained by the second law if the thermodynamic analysis is performed correctly. Moreover, the ratio of the last term to the second one is estimated as $[\Delta\Theta]/[\Theta]$, and, therefore, can be omitted within an accuracy adopted in Section 3.1. It can also be shown that the first term in expression (27) for $\hat{\Phi}_i$ can also be neglected. Following the philosophy of algebraic turbulent modelling, we approximate the second term in (27) by a diffusive form:

$$\hat{\Phi}_i = -\chi(\Theta, k, \varepsilon) S_{,i}^T, \quad (31)$$

which yields

$$\frac{\lambda}{\Theta^2} \Theta_{,i} \Theta_{,i} + \frac{2\chi}{\Theta} \Theta_{,i} S_{,i}^T + \frac{1}{\Theta} (\mu D_{(ij)} D_{(ij)} + \rho \varepsilon) + \lambda \xi \geq 0. \quad (32)$$

Evidently, with the condition that $\lambda, \mu, \varepsilon, \xi$ are non-negative, (32) finally yields a constraint for χ , because ξ , as a constitutive quantity, can generally depend on $S_{,i}^T$. This constraint, however, does not determine any additional constraint on the k - ε model, because χ does not enter it. In the case when $\chi = 0$, we derive (8) averaged with the approximation $1/\bar{\theta} \approx 1/\Theta$. It should be noted that $\hat{\Phi}_i$ enters the entropy production because we assumed a reduced form for the turbulent entropy (23). If we took the next term into account, then the part of $\hat{\Phi}_i$ describing the turbulent transfer $\overline{u_i \theta^2}$ would drop out.

The expression of the turbulent entropy (19), including the quantity $\overline{\frac{1}{2}\theta^2}$, the balance equation (29) for $\overline{\frac{1}{2}\theta^2}$ and the form of the entropy production (32), suggests the following form of an evolution equation for the turbulent entropy S^T when $[\Delta\Theta]/[\Theta] \ll 1$:

$$\rho S^{T\bullet} = \frac{\rho}{\Theta^2} Q_i^T \Theta_{,i} - \frac{1}{\Theta^2} \frac{\partial}{\partial x_i} \left(\Theta^2 \hat{\Phi}_i \right) + \lambda \xi, \quad (33)$$

where the first term describes exchange of the entropy between the mean and turbulent part, the second term describes the turbulent entropy flux, and ξ is a production term. The last term in (29) was omitted as having negligible influence on the whole entropy production when $[\Delta\Theta]/[\Theta] \ll 1$. Now, the entropy inequality (20), with the help of (19), (27) and (33), takes the form (32) and yields the same necessary and sufficient conditions of thermodynamic consistency as derived in Section 2.

4. Conclusions

It was shown that the classical version of the second law adopted in irreversible thermodynamics can be effectively applied for turbulent closure models without assumption on the form of the constitutive law for the turbulent entropy. This leads to the conclusion that a solution determined by a closure is thermodynamically consistent if it satisfies only the well-known realizability conditions. The constitutive laws for the Reynolds stresses and turbulent heat fluxes are not constrained directly by the second law, but only through the realizability conditions. Analysing the k - ε model demonstrated that application of methods of thermodynamics using a constitutive law for the turbulent entropy cannot be informative and can impose unnecessary restrictions due to the non-universality of the closure scheme. The constitutive law for the entropy found with the assumption that a turbulent flow can be considered as a flow of a multi-temperature fluid is not consistent with the second law of thermodynamics. For the case of relatively small temperature fluctuations, the correct constraints can be achieved by assuming an evolution equation for the turbulent entropy in a form suggested by the balance equation for the temperature fluctuations.

It should be noted that the above conclusions do not generally mean that methods of thermodynamics cannot be applied to developing turbulent models at all. For example, one of the applications of extended thermodynamics leading to k - ε model accounting for relaxation effects was performed by Huang and Rajagopal (1996), who, however, did not use the second law for constraining the model.

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