UNCLASSIFIED

Defense Technical Information Center
Compilation Part Notice

ADP013642

TITLE: Physics-Preserving Turbulent Closure Models

DISTRIBUTION: Approved for public release, distribution unlimited

This paper is part of the following report:

TITLE: DNS/LES Progress and Challenges. Proceedings of the Third AFOSR International Conference on DNS/LES

To order the complete compilation report, use: ADA412801

The component part is provided here to allow users access to individually authored sections of proceedings, annals, symposia, etc. However, the component should be considered within the context of the overall compilation report and not as a stand-alone technical report.

The following component part numbers comprise the compilation report:
ADP013620 thru ADP013707

UNCLASSIFIED
Abstract. Both necessary and sufficient conditions are derived in a systematic, rigorous way for a subgrid-scale (SGS) flux vector model to preserve the frame-indifference of the vector and to satisfy both the principle of material frame indifference (PMFI) and the second law of thermodynamics. This leads to the results either confirming the previous intuitive arguments or offering new insights into turbulence modelling, and is of significance in clarifying some controversies in the literature, examining how well existing models preserve the physics, and developing new models.

1. Introduction

SGS stresses and fluxes of mass and energy are believed to be quantities determined by filtered large-scale velocity and mass fraction/temperature fields in the large eddy simulation (LES). Based on this fundamental, intrinsic belief, various approaches have been proposed to relate SGS stresses and fluxes to the filtered large-scale fields, so-called SGS turbulence modelling. The readers are referred to Ciofalo (1994), Mason (1994), Lesieur & Métaias (1996) and Sagaut (2001) for some recent excellent reviews and discussions of this important topic. While some LES results based on some commonly used models seem encouraging, they fail to meet either one or both of two natural fundamental requirements for turbulence models: preserving the fundamental properties of the quantities being modeled and satisfying some classical principles.

The modelling of the SGS flux vectors of mass and energy consists of replacing them by constitutive equations expressing them as functions of filtered large-scale fields of velocity and mass fraction/temperature. While such constitutive equations may take different forms such as algebraic and differential, it appears to be a basic requirement to preserve the properties
which the flux vectors hold by their definition. Such a property is the frame-
indifference (Fureby & Tabor 1997, Ghosal 1999, Wang 2001). It follows
from the definition of the SGS flux vectors and states that they remain the
same directed line element under a change of frame. The issue concerned
with whether a model guarantees this property is referred as the invariance
in the literature.

While the first requirement focuses on the properties of the SGS flux
vectors themselves, the second requirement emphases on their function rela-
tion with the filtered large-scale fields. Such function relations are required
to satisfy some classical principles including the PMFI and the second law
2001). The PMFI requires that the function relation is the same for every
observer, i.e. in every frame of reference. The second law of thermodynam-
ics, on the other hand, states that the flux is always from high concentration
to low concentration. Note that the realizability for the Reynolds and SGS
stresses also comes from the second law of thermodynamics (Wang 1999,
2001).

The motivation for the present work comes from the desire to derive
both necessary and sufficient condition in a systematic, rigorous way for a
SGS flux model to preserve the frame-indifference of SGS flux vectors and
to satisfy both the PMFI and the second law of thermodynamics. Unlike
the works in the literature, no intuitive assumption is introduced in the
derivation; the independent variables are chosen properly; the PMFI and
the frame indifference of SGS flux vectors are clearly distinguished. This
leads to some conclusive results. Among them, some confirm the previ-
ous intuitive arguments, and others form new insights to SGS turbulence
modelling.

2. Principle of Material Frame-Indifference and Second Law of
Thermodynamics

Consider a class of constitutive relations which relate the passive SGS flux
vector $q$ of mass or energy to its arguments $\theta, O.P., \nabla \theta, v, L$, i.e.,

$$q = f(\theta, O.P., \nabla \theta, v, L). \tag{1}$$

Here $f$ is a vector-valued function. $\theta$ is the concentration of a property.
It is the mass fraction of a species for the case of SGS flux of mass, and
the temperature when $q$ is the SGS flux of energy. $O.P.$ denotes the other
scalar-valued thermophysical parameters which are independent of $v$ and
$L$ and are typically the local thermodynamic state variables. $\nabla \theta$ is the
gradient of $\theta$. $v$ is the filtered velocity vector. $L$ is the velocity gradient
tensor of $v$, a second order tensor-valued variable.
In sharp contrast with that in the literature, we choose $L$ as an independent variable instead of its symmetric part $D$ (the velocity strain tensor) and skew part $W$ (the vorticity tensor) because $D$ and $W$ can not be regarded as independent. We do not include $k$, $l$ or $\varepsilon$ as the independent variables. The exclusion of the explicit dependence of $q$ on time $t$ and position vector $r$ comes from the fact that they affect $q$ through $\theta$, $O.P.$, $\nabla \theta$, $v$ and $L$.

The relation (1) satisfies both principle of determinism and principle of local action since we assume that $q$ at a point and a time instant is a function of its arguments at that point and that instant.

The principle of frame-indifference requires that $f$ is the same for every observer, i.e.,

$$q^* = f(\theta^*, O.P.*, (\nabla \theta^*)^*, v^*, L^*)$$

in which superscript $*$ represents the quantities observed by another observer $*$. 

The second law of thermodynamics states that $q$ is always from high concentration to low concentration. This requires that: (1) $f$ changes its sign if $V^0$ changes the sign, i.e.,

$$f(\theta, O.P., -V^0, v, L) = -f(\theta, O.P., \nabla \theta, v, L),$$

and (2) the projection of the $f$ on $\nabla \theta$ is negative semi-definite, i.e.,

$$f \cdot \nabla \theta \leq 0.$$ 

2.1. NECESSARY CONDITIONS FOR REQUIREMENTS (2) AND (3)

2.1.1. $q - v$ relation

Theorem 1. $f$ is independent of $v$.

Proof From the principle of observer transformations (Geankoplis 1983, Truesdell 1991),

\[
\begin{align*}
\theta^* &= \theta, \\
(O.P.)^* &= O.P., \\
(\nabla \theta^*)^* &= Q(t) \nabla \theta, \\
L^* &= Q(t) L Q^T(t) + \dot{Q}(t) Q^T(t), \\
r^* &= Q(t)r + c(t), \\
v^* &= \frac{d r^*}{dt} = Q(t)r + Q(t) v + \dot{c}(t),
\end{align*}
\]

where $Q$ is an arbitrary rotation tensor, $r$ a position vector of material point, $c(t)$ an arbitrary vector-valued function of time $t$, and a dot over a letter indicates a time derivative. In (5), we have used the frame indifference of $q$. 
By making use of (1) and (5), (2) yields (suppressing \( t \))

\[
f(\theta, O.P., Q\nabla \theta, Qr + Qv + \dot{c}, QLqT + \dot{Q}Q^T) = Qf(\theta, O.P., \nabla \theta, v, L),
\forall Q \text{ and } c.
\]

(6)

Since (6) holds for all \( Q \), it must be true for \( Q = 1 \). Take \( Q = 1 \), then \( \dot{Q} = 0 \). Equation (6) reduces to

\[
f(\theta, O.P., \nabla \theta, v + \dot{c}, L) = f(\theta, O.P., \nabla \theta, v, L) \quad \forall \dot{c}.
\]

(7)

This implies that \( f \) is independent of velocity \( v \).

By applying Theorem 1, (1) and (6) reduce to

\[
q = f(\theta, O.P., vo, L),
\]

(8)

\[
f(\theta, O.P., Q\nabla \theta, QLQ^T + \dot{Q}Q^T) = Qf(\theta, O.P., \nabla \theta, L) \quad \forall Q.
\]

(9)

2.1.2. \( q - L \) relation

Note that \( L \) can be uniquely decomposed into a symmetric tensor \( D \) (velocity strain tensor) and a skew tensor \( W \) (vorticity tensor). Expression (9) may, then, be rewritten as

\[
f(\theta, O.P., Q\nabla \theta, QDQ^T + QWQ^T + \dot{Q}Q^T) = Qf(\theta, O.P., \nabla \theta, L) \quad \forall Q.
\]

(10)

**Theorem 2.** For rotation tensor \( Q(t) = \exp[\dot{\Omega}(t - \tau)]\dot{Q} \), we can, at any instant \( \tau \), pick \( Q(\tau) \) and \( Q(\tau)Q^T(\tau) \) to be arbitrary, independent rotation and skew tensors, respectively. Here \( \dot{Q} \) is any time-independent rotation tensor, and \( \dot{\Omega} \) any time-independent skew tensor.

**Proof** As \( \dot{\Omega} \) is a time-independent skew tensor, \( \exp[\dot{\Omega}(t - \tau)] \) is thus a rotation tensor for any fixed time \( \tau \) and all time \( t \). Since both \( \dot{Q} \) and \( \exp[\dot{\Omega}(t - \tau)] \) are rotation tensors, \( Q(t) = \exp[\dot{\Omega}(t - \tau)]\dot{Q} \) is also a rotation tensor for all time \( t \). Also,

\[
Q(\tau) = \dot{Q}.
\]

(11)

\[
\dot{Q}(\tau)Q^T(\tau) = \dot{\Omega}Q(\tau)Q^T(\tau) = \dot{\Omega}.
\]

(12)

They are clearly independent rotation and skew tensors if \( \dot{Q} \) and \( \dot{\Omega} \) are any time-independent rotation and skew tensors, respectively.

**Theorem 3.** \( L \) affects \( q \) only through velocity strain tensor \( D \).

**Proof** To prove this, choose \( Q(t) \) defined in Theorem 2 as the rotation tensor in (10) while for any instant \( \tau \), \( -QWQ^T |_{\tau} \) is used as the skew
tensor $\Omega$, i.e. $\Omega = -QWQ^T |_{\tau}$ (Such a $\Omega$ do a skew tensor since $\Omega^T = -QW^TQ^T |_{\tau} = QWQ^T |_{\tau} = -\Omega$). Then at time $t = \tau$, (10) yields

$$f(\theta, O.P., Q\nabla\theta, QDQ^T) = \dot{Q}f(\theta, O.P., \nabla\theta, L) \quad \forall Q.$$  

(13)

As this is true for all rotation tensor $\dot{Q}$, it must hold for $\dot{Q} = 1$. Let $\dot{Q} = 1$, (13) yields

$$f(\theta, O.P., \nabla\theta, L) = f(\theta, O.P., \nabla\theta, D),$$  

(14)

or

$$q = f(\theta, O.P., \nabla\theta, D).$$  

(15)

2.1.3. $q-\nabla\theta$ relation

Expression (15) and the principle of frame-indifference together yield

$$q^* = f(\theta^*, (O.P.)^*, (\nabla\theta^*)^*, D^*)$$  

(16)

By making use of (5), (15) and $D^* = QDQ^T$ (Truesdell 1991), (16) leads to

$$f(\theta, O.P., Q\nabla\theta, QDQ^T) = Qf(\theta, O.P., \nabla\theta, D) \quad \forall Q.$$  

(17)

Also the second law of thermodynamics [Eq.(3)] requires that

$$f(\theta, O.P., -\nabla\theta, D) = -f(\theta, O.P., \nabla\theta, D).$$  

(18)

Since the velocity strain tensor $D$ is a real, symmetric tensor, it has three real eigenvalues. The three eigenvalues can be distinct, identical, or two of them can be identical. In the present work, we focus on the case that the three eigenvalues are distinct. Similar results may be obtained for the other two cases.

**Theorem 4.** $\nabla\theta, D, D^2, \nabla\theta$ are linearly independent if three eigenvalues of $D$ are distinct.

**Proof** Let $\mu_k$ and $f_k$ ($k = 1, 2, 3$) to be the eigenvalues and eigenvectors of $D$. $D$ may be represented, in its spectral form, as

$$D = \sum_{k=1}^{3} \mu_k f_k \otimes f_k.$$  

(19)

The linear independence of $f_k$ ($k = 1, 2, 3$) allows us to write $\nabla\theta$ as

$$\nabla\theta = (\nabla\theta)_j f_j$$  

(20)

in which $(\nabla\theta)_j = \nabla \cdot f_j$. 


Suppose that $\nabla \theta, D \nabla \theta$ and $D^2 \nabla \theta$ are linearly dependent for all $D$ and $\nabla \theta$, there are $\alpha, \beta$ and $\gamma$ which are not all zero, such that
\[ \alpha \nabla \theta + \beta D \nabla \theta + \gamma D^2 \nabla \theta = 0. \] (21)
Substituting (19) and (20) into (21) yields
\[ \sum_{k=1}^{3} (\alpha + \beta \mu_k + \gamma \mu_k^2) (\nabla \theta)_k f_k = 0, \] (22)
which implies, as $f_k$ $(k = 1, 2, 3)$ are linearly independent,
\[ (\alpha + \beta \mu_k + \gamma \mu_k^2) (\nabla \theta)_k = 0, \quad (k = 1, 2, 3). \] (23)
For arbitrary $\nabla \theta$, $(\nabla \theta)_k$ need not be zero, so
\[ \alpha + \beta \mu_k + \gamma \mu_k^2 = 0, \quad (k = 1, 2, 3) \] (24)
that requires that $\alpha = \beta = \gamma = 0$ for distinct $\mu_k$, contrary to the hypothesis. Theorem 4 has, thus, been proved.

Applying Theorem 4 to the SGS flux vector, we have
\[ f(\theta, O.P., \nabla \theta, D) = \phi_0(\theta, O.P., \nabla \theta, D) \nabla \theta + \phi_1(\theta, O.P., \nabla \theta, D) D \nabla \theta + \phi_2(\theta, O.P., \nabla \theta, D) D^2 \nabla \theta, \] (25)
and
\[ f(\theta, O.P., -\nabla \theta, D) = -\phi_0(\theta, O.P., -\nabla \theta, D) \nabla \theta - \phi_1(\theta, O.P., -\nabla \theta, D) D \nabla \theta - \phi_2(\theta, O.P., -\nabla \theta, D) D^2 \nabla \theta. \] (26)
Substituting (25) and (26) into (18) leads to
\[ [\phi_0(\theta, O.P., \nabla \theta, D) - \phi_0(\theta, O.P., -\nabla \theta, D)] \nabla \theta + [\phi_1(\theta, O.P., \nabla \theta, D) - \phi_1(\theta, O.P., -\nabla \theta, D)] D \nabla \theta + [\phi_2(\theta, O.P., \nabla \theta, D) - \phi_2(\theta, O.P., -\nabla \theta, D)] D^2 \nabla \theta = 0 \] (27)
which implies, since $\nabla \theta, D \nabla \theta$ and $D^2 \nabla \theta$ are linearly independent,
\[ \phi_i(\theta, O.P., \nabla \theta, D) = \phi_i(\theta, O.P., -\nabla \theta, D), \quad (i = 0, 1, 2). \] (28)
To satisfy this requirement, take
\[ \phi_i(\theta, O.P., \nabla \theta, D) = \psi_i(\theta, O.P., \nabla \theta \otimes \nabla \theta, D), \quad (i = 0, 1, 2). \] (29)
Then (25) and (29) result in
\[ f(\theta, O.P., Q \nabla \theta, QDQ^T) = Q(\hat{\psi}_0 \nabla \theta + \hat{\psi}_1 D \nabla \theta + \hat{\psi}_2 D^2 \nabla \theta) \] (30)
in which,
\[ \psi_i = \psi_i(\theta, O.P., Q\nabla\theta \otimes Q\nabla\theta, QDQ^T), \]
and
\[ Qf(\theta, O.P., \nabla\theta, D) = Q(\psi_0 \nabla\theta + \psi_1 D \nabla\theta + \psi_2 D^2 \nabla\theta). \] (31)

By making use of (30) and (31), (17) yields
\[ (\hat{\psi}_0 - \psi_0)\nabla\theta + (\hat{\psi}_1 - \psi_1)D \nabla\theta + (\hat{\psi}_2 - \psi_2)D^2 \nabla\theta = 0 \] (32)
that implies, by Theorem 4,
\[ \psi_i(\theta, O.P., Q\nabla\theta \otimes Q\nabla\theta, QDQ^T) = \psi_i(\theta, O.P., \nabla\theta \otimes \nabla\theta, D) \quad \forall Q. \] (33)

**Theorem 5.** Suppose
\[ \psi(\theta, O.P., Qb \otimes Qb, QBQ^T) = \psi(\theta, O.P., b \otimes b, B), \quad \forall b \text{ and } B, \]
then
\[ \psi(\theta, O.P., a \otimes a, A) = \psi(\theta, O.P., b \otimes b, B) \]
whenever \( J_k(a, A) = J_k(b, B) \) \((k = 1, 2, \ldots, 6)\). Here
\[ J_1(a, A) = trA, \quad J_2(a, A) = \frac{1}{2}[(trA)^2 - tr(A^2)], \quad J_3(a, A) = detA, \quad J_4(a, A) = a \cdot Aa, \quad J_5(a, A) = a \cdot A^2a, \quad J_6(a, A) = |a|, \]
a and b are two arbitrary vectors, A and B are two arbitrary symmetric tensors.

**Proof** Since \( J_k(a, A) = J_k(b, B) \) \((k = 1, 2, 3)\), tensors A and B have same eigenvalues. Let \( \mu_k \) be their eigenvalues, A and B may be written as,
\[ A = \sum_{k=1}^{3} \mu_k e_k \otimes e_k, \quad B = \sum_{k=1}^{3} \mu_k f_k \otimes f_k \]
where \( e_k \) and \( f_k \) \((k = 1, 2, 3)\) are eigenvectors of A and B, respectively. Define
\[ Q = e_k \otimes f_k \]
that is a rotation tensor, and
\[ e_i = Qf_i, \quad A = QBQ^T, \quad A^2 = QB^2Q^T, \quad (i = 1, 2, 3). \] (34)
By applying \( J_k(a, A) = J_k(b, B) \) \((k = 4, 5, 6)\), we have
\[ \sum_{k=1}^{3} (b \cdot f_k)^2 = \sum_{k=1}^{3} (Q^T a \cdot f_k)^2, \quad \sum_{k=1}^{3} \mu_k (b \cdot f_k)^2 = \sum_{k=1}^{3} \mu_k (Q^T a \cdot f_k)^2, \]
\[ \sum_{k=1}^{3} \mu_k^2 (b \cdot f_k)^2 = \sum_{k=1}^{3} \mu_k^2 (Q^T a \cdot f_k)^2. \] (35)
This implies, for the distinct \( \mu_k \) \((k = 1, 2, 3)\),

\[
(Q^T a \mp b) \cdot f_k = 0, \quad (k = 1, 2, 3).
\]  

(36)

Note that \( f_k \) \((k = 1, 2, 3)\) are linearly independent, then \( a = \pm Q\mathbf{b}, \quad a \otimes a = Q\mathbf{b} \otimes Q\mathbf{b} \). By hypothesis,

\[
\psi(\theta, O.P., b \otimes b, B) = \psi(\theta, O.P., Q\mathbf{b} \otimes Q\mathbf{b}, QBQ^T) = \psi(\theta, O.P., a \otimes a, A)
\]

in which \( A = QBQ^T \) [ (34)] and \( a \otimes a = Q\mathbf{b} \otimes Q\mathbf{b} \) are used. Therefore,

\[
\psi(\theta, O.P., b \otimes b, B) = \psi[\theta, O.P., J_k(b, B)], \quad (k = 1, 2, \cdots, 6)
\]  

(37)

if

\[
\psi(\theta, O.P., Q\mathbf{b} \otimes Q\mathbf{b}, QBQ^T) = \psi(\theta, O.P., b \otimes b, B), \quad \forall \mathbf{b} \text{ and } B. \quad (38)
\]

The converse is also true since \( J_k(Q\mathbf{b}, QBQ^T) = J_k(b, B) \) \((k = 1, 2, \cdots, 6)\).

**Theorem 6.** The necessary condition for the constitutive process (1) to satisfy requirements (2) and (3) is

\[
q = f(\theta, O.P., \nabla \theta, D) = (\phi_0 1 + \phi_1 D + \phi_2 D^2) \nabla \theta
\]

where

\[
\phi_i = \phi_i[\theta, O.P., J_k(\nabla \theta, D)], \quad (i = 0, 1, 2; \quad k = 1, 2, \cdots, 6).
\]

**Proof** Applying Theorem 5 to (33) yields

\[
\psi_1(\theta, O.P., \nabla \theta \otimes \nabla \theta, D) = \psi_1[\theta, O.P., J_k(\nabla \theta, D)]. \quad (39)
\]

This, with (25) and (29), leads to

\[
q = f(\theta, O.P., \nabla \theta, D) = (\phi_0 1 + \phi_1 D + \phi_2 D^2) \nabla \theta
\]  

(40)

where

\[
\phi_i = \phi_i[\theta, O.P., J_k(\nabla \theta, D)], \quad (i = 0, 1, 2; \quad k = 1, 2, \cdots, 6).
\]

If the three eigenvalues of \( D \) are not distinct, we can still obtain (40) with \( \phi_1 = \phi_2 = 0 \) (for the case of three identical eigenvalues) or \( \phi_2 = 0 \) (for the case of two identical eigenvalues) by the similar method. Therefore, (40) is valid for all cases.
2.2. SUFICIENCY OF (40) FOR REQUIREMENTS (2) AND (3)

Suppose (40) holds, then

\[
\begin{align*}
\mathbf{f}(\theta^*, \mathbf{O.P.}^*, (\nabla \theta^*)^*, \mathbf{v}^*, \mathbf{L}^*) &= \{\phi_0(\theta^*, \mathbf{O.P.}^*, J_k((\nabla \theta^*)^*, \mathbf{D}^*)) \mathbf{1} \\
&+ \phi_1(\theta^*, \mathbf{O.P.}^*, J_k((\nabla \theta^*)^*, \mathbf{D}^*)) \mathbf{D}^* + \phi_2(\theta^*, \mathbf{O.P.}^*, J_k((\nabla \theta^*)^*, \mathbf{D}^*)) \mathbf{D}^{*2}\}
\end{align*}
\]

\[
(\nabla \theta^*)^* = \{\phi_0(\theta, \mathbf{O.P.}, J_k(\mathbf{Q} \nabla \theta, \mathbf{QDQ^T})) \mathbf{Q1}^T + \phi_1(\theta, \mathbf{O.P.}, J_k(\mathbf{Q} \nabla \theta, 
\mathbf{QDQ^T}))) \mathbf{QDQ^T} + \phi_2(\theta, \mathbf{O.P.}, J_k(\mathbf{Q} \nabla \theta, \mathbf{QDQ^T})) \mathbf{D}^2 \mathbf{Q}^T\} \mathbf{Q} \nabla \theta
\]

\[
\begin{align*}
\mathbf{D}^* &= \mathbf{QDQ^T} \\
J_k(\mathbf{Q} \nabla \theta, \mathbf{QDQ^T}) &= J_k(\mathbf{Q} \nabla \theta, \mathbf{D}) (k = 1, 2, \ldots, 6)
\end{align*}
\]

(41)

in which Eq.(5), \( \mathbf{D}^* = \mathbf{QDQ^T} \) and \( J_k(\mathbf{Q} \nabla \theta, \mathbf{QDQ^T}) = J_k(\nabla \theta, \mathbf{D}) (k = 1, 2, \ldots, 6) \) are used.

Also, if (40) holds,

\[
\begin{align*}
\mathbf{f}(\theta, \mathbf{O.P.}, - \nabla \theta, \mathbf{v}, \mathbf{L}) &= \{\phi_0(\theta, \mathbf{O.P.}, J_k(- \nabla \theta, \mathbf{D})) \mathbf{1} \\
&+ \phi_1(\theta, \mathbf{O.P.}, J_k(- \nabla \theta, \mathbf{D})) \mathbf{D} + \phi_2(\theta, \mathbf{O.P.}, J_k(- \nabla \theta, \mathbf{D})) \mathbf{D}^2\}(- \nabla \theta)
\end{align*}
\]

\[
= -\{\phi_0(\theta, \mathbf{O.P.}, J_k(\nabla \theta, \mathbf{D})) \mathbf{1} + \phi_1(\theta, \mathbf{O.P.}, J_k(\nabla \theta, \mathbf{D})) \mathbf{D} + \phi_2(\theta, \mathbf{O.P.}, J_k(\nabla \theta, \mathbf{D})) \mathbf{D}^2\}(\nabla \theta) = -\mathbf{f}(\theta, \mathbf{O.P.}, \nabla \theta, \mathbf{v}, \mathbf{L}) (k = 1, 2, \ldots, 6)
\]

(42)

in which \( J_k(- \nabla \theta, \mathbf{D}) = J_k(\nabla \theta, \mathbf{D}) (k = 1, 2, \ldots, 6) \) are used. Equations (41) and (42) establish the sufficiency of (40) for (2) and (3).

2.3. PROPERTIES OF \( \phi_i \) (\( i = 0, 1, 2 \)) AND BOTH NECESSARY AND SUFFICIENT CONDITIONS FOR INEQUALITY (4)

Both necessity and sufficiency of (40) for Eqs.(2) and (3) are established in §2.1 and §2.2. Here we analyze some fundamental properties of \( \phi_i \) (\( i = 0, 1, 2 \)), and develop both necessary and sufficient conditions for inequality (4).

Rewrite Eq.(40) as

\[
\mathbf{q} = -\mathbf{K} \nabla \theta,
\]

(43)

with

\[
\mathbf{K} = -(\phi_0 \mathbf{1} + \phi_1 \mathbf{D} + \phi_2 \mathbf{D}^2) = \phi_0 \mathbf{1} + \phi_1 \mathbf{D} + \phi_2 \mathbf{D}^2.
\]

(44)

Here \( \mathbf{1} \) is a unit (identity) tensor, and

\[
\phi_i = -\phi_i \quad (i = 0, 1, 2).
\]

(45)

\( \mathbf{K} \) has two fundamental properties: (1) it is a real-valued tensor on the ground of practical transport processes, and (2) it is a symmetric tensor due to the symmetry of velocity strain tensor \( \mathbf{D} \).
Let $\lambda_j$ and $f_j \ (j = 1, 2, 3)$ be the three eigenvalues of $D$ and $K$, respectively. Since $K$ is related to $D$ through Eq.(44),

$$f_j = \varphi_0 + \varphi_1 \lambda_j + \varphi_2 \lambda_j^2, \quad (j = 1, 2, 3). \quad (46)$$

Because $D$ and $K$ are real-valued symmetric tensors, $\lambda_j$ and $f_j \ (j = 1, 2, 3)$ must be real-valued, i.e.,

$$f_j = \bar{f}_j, \quad (j = 1, 2, 3), \quad (47)$$

$$\bar{\lambda}_j = \lambda_j, \quad (j = 1, 2, 3). \quad (48)$$

By Eq.(46),

$$\bar{f}_j = \varphi_0 + \varphi_1 \bar{\lambda}_j + \varphi_2 \bar{\lambda}_j^2, \quad (j = 1, 2, 3). \quad (49)$$

By making use of Eqs.(47) and (48), Eq.(49) leads to

$$f_j = \bar{\varphi}_0 + \varphi_1 \lambda_j + \varphi_2 \lambda_j^2, \quad (j = 1, 2, 3). \quad (50)$$

This, with Eq.(46), yields

$$(\varphi_0 - \bar{\varphi}_0) + (\varphi_1 - \bar{\varphi}_1) \lambda_j + (\varphi_2 - \bar{\varphi}_2) \lambda_j^2 = 0, \quad (j = 1, 2, 3), \quad \forall \lambda_j \in R \quad (51)$$

which indicates that

$$\varphi_i = \bar{\varphi}_i, \quad (i = 0, 1, 2). \quad (52)$$

Therefore, $\varphi_i \ (i = 0, 1, 2)$ must be real-valued.

Substituting Eq.(43) into inequality (4) yields

$$\nabla\theta \cdot K \nabla\theta \geq 0, \quad \forall \nabla\theta, \quad (53)$$

which implies that $K$ is positive semi-definite. Note also that $K$ is, in practice, an invertible tensor, it must be positive definite. The same conclusion may be obtained by noting that the equal sign in (4) is only for reversible processes and transport processes are irreversible.

The necessary and sufficient condition for a symmetric tensor to be positive definite is that all of its eigenvalues are positive definite. Both necessary and sufficient condition for inequality (4) is, thus,

$$\varphi_0 + \varphi_1 \lambda_j + \varphi_2 \lambda_j^2 > 0, \quad (j = 1, 2, 3), \quad \forall \lambda_j \in R. \quad (54)$$

Two necessary conditions of (54) can be easily obtained by considering cases of $\lambda_j = 0$ and $|\lambda_j| \to \infty$, respectively, as

$$\varphi_0 > 0, \quad (55)$$
\[ \varphi_2 > 0. \]  

(56)

Dividing (54) by \( \varphi_0 \), we can rearrange (54) into an alternative form

\[
(1 + \frac{\varphi_1 \lambda_j}{2 \varphi_0})^2 + \left( \frac{\varphi_2}{\varphi_0} - \frac{\varphi_1^2}{4 \varphi_0^2} \right) \lambda_j^2 > 0 \quad \forall \lambda_j \in R. 
\]

(57)

This yields another necessary condition, by setting \( \lambda_j = -2 \varphi_0 / \varphi_1 \),

\[
\varphi_1^2 - 4 \varphi_0 \varphi_2 < 0. 
\]

(58)

Conversely, it is easy to show that (55), (56) and (58) are also the sufficient conditions of (54).

The detailed expressions of \( \varphi_0, \varphi_1 \) and \( \varphi_2 \) are material-dependent and need to be determined through experiments. Once they are determined, Eq. (43) can serve as the SGS flux model that is properly invariant and satisfies the second law of thermodynamics.

3. Concluding Remarks

For a class of turbulence flows for which the SGS flux vector can be described by Eq.(1), both necessary and sufficient conditions are derived in a systematic, rigorous way for the invariance, the PMFI and the second law of thermodynamics. This leads to a general model (43) with three real-valued functions \( \varphi_i \) \((i = 0, 1, 2)\) satisfying (55) (56) and (58). Any specific model satisfying (43), (55), (56) and (58) is properly invariant and satisfies the second law of thermodynamics while the model violating these conditions is not. The work is believed to be important both for developing the specific, physics-preserving models and for clarifying some confusion in the literature by noting that the previous works employ an intuitive approach with the focus on only obtaining the sufficient condition.

Acknowledgments: Financial support from the Outstanding Young Researcher Award 2000-2001, the CRCG of the University of Hong Kong is gratefully acknowledged.

References


