

# Continuum Thermo-Mechanics Fundamentals

James R. Rice, notes prepared Nov and Dec 2009  
(graphics inserted Oct 2017 by Paul Le Floch)  
for Engineering Sciences 220, Fluid Dynamics, at Harvard University

## Conserved Quantities

Let a conserved quantity have amount  $F$  per unit volume. Examples are as follows:

For conservation of **mass**, we take  $F = \rho$ , where  $\rho$  is mass density.

For conservation of **linear momentum**,  $F = \rho \mathbf{u}$ , where  $\mathbf{u}$  is the velocity vector (relative to some Newtonian reference frame).

For conservation of **angular momentum**,  $F = \rho \mathbf{x} \times \mathbf{u}$ , where  $\mathbf{x}$  is the position vector (relative to a fixed point in that frame).

For conservation of **energy** (first law of thermodynamics),  $F = \rho (e + \frac{1}{2}|\mathbf{u}|^2)$  where  $e$  is the internal energy per unit mass and  $\frac{1}{2}|\mathbf{u}|^2$  is the kinetic energy per unit mass.

There is also the non-conservation law of **entropy** (second law of thermodynamics) for which the same framework here will be used, replacing an “=” with a “ $\geq$ ”, and in which  $F = \rho s$  where  $s$  is entropy per unit mass.

We assume that at the continuum scales of interest here, the mass density  $\rho$  as well as the the momentum per unit volume  $\rho \mathbf{u}$  can be interpreted as well-defined averages of microscopic masses and momenta. That is, they are averages over minute spatial regions and time intervals, which can nevertheless be chosen large enough that there are negligible statistical fluctuations about those averages at a given  $\mathbf{x}, t$  in different macroscopic realizations of the same deformation or flow process. Accordingly,  $\mathbf{u}$  must then be interpreted as the *mass averaged* velocity. When studying the motion of a surface  $S$  in the continuum which is said to *move with the material*, we will interpret that as moving with the local velocity  $\mathbf{u}$ . Correspondingly, then, in writing the law of conservation of, e.g., linear momentum for a region of material momentarily occupying volume  $V$ , the surface flux rate of momentum  $\mathbf{T}$  (where  $\mathbf{T}$  is the *stress vector* along the bounding surface  $S$  of  $V$ ), is understood to include contributions not just from forces acting on  $S$  but *also* from transfers of momentum across  $S$  associated with microscopic scale motions relative to the mass-averaged motion  $\mathbf{u}$ .

We consider a single-component continuum. More complicated expressions than given here would be required to describe multi-component continua in which one component moves macroscopically relative to the other(s), like for fluids entraining solid particles or droplets of other fluids, or for deformable porous solids with fluid infiltration, etc.

## Representation of Accumulation Rates in Conservation Laws; Reynolds Transport Theorem

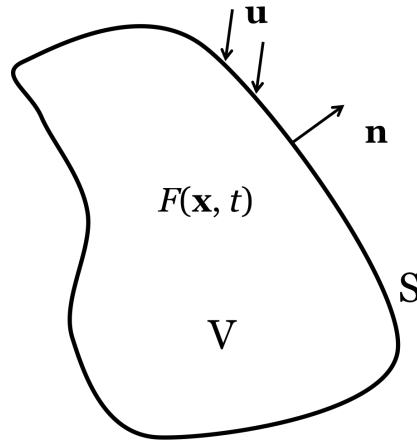


Figure 1: An arbitrarily selected volume  $V$  of space, with bounding surface  $S$ .

We use Eulerian coordinates (fixed in space) so, focusing attention on an arbitrarily selected volume  $V$  of space, with bounding surface  $S$ . Conservation laws have the form:

$$\begin{aligned} & \text{Rate of accumulation of quantity } F \text{ within the matter which, at time } t, \text{ occupies region } V \\ &= \text{Rate of generation of that quantity within } V \text{ and along its surface } S \end{aligned}$$

Because of the Eulerian coordinates, to properly judge the *rate of accumulation* of  $F$ , we must account for the change within  $V$  as well as for the fact that some of the matter within  $V$  at time  $t$  will, at an infinitesimally later time  $t + \delta t$ , have exited  $V$  across  $S$  at locations where  $\mathbf{n} \cdot \mathbf{u} > 0$  (here  $\mathbf{n}$  is the outer unit normal to  $S$ ), and that other matter will have entered  $V$  through  $S$  at places where  $\mathbf{n} \cdot \mathbf{u} < 0$ . (Had we used Lagrangian coordinates (i.e., fixed along material points), the terms crossing  $S$  would not appear and, rather, we'd say that the boundary of  $V$  moves with velocity  $\mathbf{u}$ .) Hence, with the Eulerian description,

$$\begin{aligned} & \text{Accumulation of quantity in } V \text{ within time } \delta t \\ &= \int_V [F(\mathbf{x}, t + \delta t) - F(\mathbf{x}, t)] dV + \int_S F(\mathbf{x}, t) (\mathbf{n} \cdot \mathbf{u} \delta t) dS \end{aligned}$$

to first order in  $\delta t$ . Dividing by  $\delta t$  and letting  $\delta t \rightarrow 0$ , this shows that

$$\text{Rate of accumulation of quantity in } V = \int_V \frac{\partial F}{\partial t} dV + \int_S \mathbf{n} \cdot \mathbf{u} F dS = \int_V \left( \frac{\partial F}{\partial t} + \nabla \cdot (\mathbf{u} F) \right) dV$$

where the *Divergence Theorem* has been used in the last step. So we simply choose  $F = \rho$ , or  $\rho \mathbf{u}$ , or  $\rho \mathbf{x} \times \mathbf{u}$ , or  $\rho(e + \frac{1}{2}|\mathbf{u}|^2)$  to get the left side of the conservation law for the respective

cases of mass, linear momentum, angular momentum, and energy. (The result of the above calculation, e.g., when rewritten as

$$\frac{d}{dt} \int_{V(t)} F dV = \int_V \left( \frac{\partial F}{\partial t} + \nabla \cdot (\mathbf{u}F) \right) dV ,$$

is sometimes referred to as the *Reynolds transport theorem*.)

## Representation of Generation Rates in Conservation Laws

The form taken by the *generation rate* will, if non-zero, be of the form

$$\text{Generation rate} = \int_V H dV + \int_S h_n dS$$

Thus, in *integral* form, each conservation law will read

$$\int_V \left( \frac{\partial F}{\partial t} + \nabla \cdot (\mathbf{u}F) \right) dV = \int_V H dV + \int_S h_n dS .$$

The physical dimensions of  $H$  and  $h_n$ , as monomials in mass (M), length (L) and time (T), must evidently satisfy  $\dim[H] = \dim[F]/T$  and  $\dim[h_n] = \dim[F]L/T$ . Also,  $H$  and  $h_n$  must have the *same tensorial rank* as does  $F$ .

## Tensors Associated with Surface Fluxes

An important conclusion may now be drawn, from the conservation law itself, about the allowable form of any surface generation term  $h_n$ : Divide both sides of the last equation by the total surface area  $S$  of the region, and then let  $S \rightarrow 0$  and  $V \rightarrow 0$  in such a way that the greatest linear dimension of  $V$  also  $\rightarrow 0$  (i.e.,  $V$  and  $S$  shrink onto a point). In that limit the volume integrals scale with  $V$  and do not contribute in the statement of the conservation law because  $V/S \rightarrow 0$ . Thus

$$\frac{1}{S} \int_S h_n dS \rightarrow 0 \quad \text{as } S \rightarrow 0 .$$

Now, in this limit, as  $V$  and  $S$  are shrunk onto a point, the quantity  $h_n$  can only vary with the orientation  $\mathbf{n}$  of the surface element at that point. The *Cauchy tetrahedron* argument then requires that for general  $\mathbf{n}$  ( $= n_1, n_2, n_3$ ), the value  $h_n$  on a surface element of that orientation has the form

$$h_n = n_1 h^{(1)} + n_2 h^{(2)} + n_3 h^{(3)} \equiv n_k h^{(k)}$$

Here  $h^{(1)}$ ,  $h^{(2)}$  and  $h^{(3)}$  are the values of  $h_n$  for surface elements with normals  $\mathbf{n}$  pointing, respectively, in the positive 1, 2, and 3 directions. This result suffices for us to conclude that the quantity  $h$  defined by

$$h = \mathbf{e}_1 h^{(1)} + \mathbf{e}_2 h^{(2)} + \mathbf{e}_3 h^{(3)} \equiv \mathbf{e}_k h^{(k)} \quad (\text{with } h_n = \mathbf{n} \cdot h)$$

is a dyad (hence has components following tensor transformation laws) having a tensorial rank which is higher by unity than the rank of  $F$ ,  $H$ , and  $h_n$ .

[For example, in the case of conservation of linear momentum,  $F$ ,  $H$ , and  $h_n$  are of rank 1, i.e., are vectors, so that  $h$  (the stress tensor) is of rank 2. In the case of conservation of energy,  $F$ ,  $H$ , and  $h_n$  are of rank 0, i.e., they are scalars, so that  $h$  (one term of which is the heat flux vector) is of rank 1.]

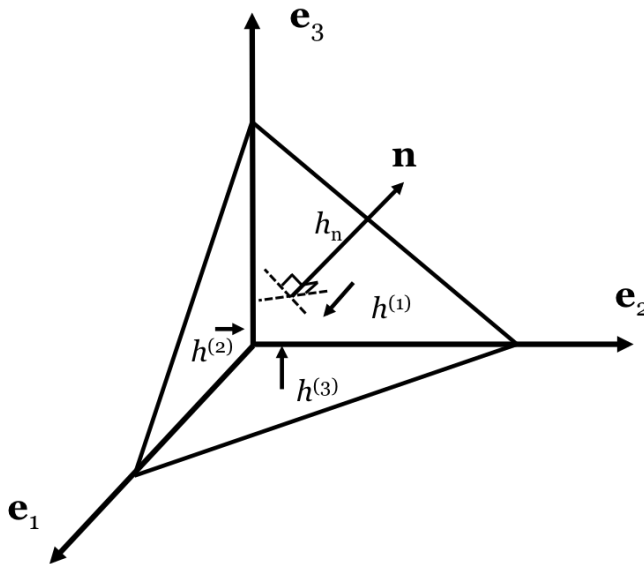


Figure 2: Cauchy tetrahedron.

### Local Form of a Conservation Law

Thus in the above integral form of a conservation law, the term  $\int_S h_n dS$  may now be rewritten as  $\int_S \mathbf{n} \cdot h dS = \int_V \nabla \cdot h dV$  by the divergence theorem. Therefore, if the conservation law applies *for any choice of V* and if the terms within it are assumed to be locally continuous, then the local (pde) form of the conservation law is [with notation  $(\dots)_{,t} \equiv \partial(\dots)/\partial t$ ]

$$F_{,t} + \nabla \cdot (\mathbf{u}F) = \nabla \cdot h + H$$

The conservation laws now follow.

#### Mass:

In the case of mass,  $F = \rho$  and there will be no generation rate,  $H = h_n = 0$ . Thus

$$\rho_{,t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

This may be rearranged to

$$\rho_{,t} + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} = 0 \quad \text{or} \quad \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0$$

where  $D(\dots)/Dt \equiv (\dots)_{,t} + \mathbf{u} \cdot \nabla(\dots)$  is the short notation for a rate of change following a material particle moving with velocity  $\mathbf{u}$ .

### Linear Momentum:

Linear momentum, for which  $F = \rho \mathbf{u}$ , is generated by force, which may be divided, according to the Cauchy stress hypothesis, into a force  $\rho \mathbf{g}$  per unit volume within  $V$  and by a force per unit area acting along  $S$ . The sum of that force per unit area on  $S$  *plus* the contribution already noted from momentum flux per unit area associated with microscopic motions relative to the mass-averaged velocity  $\mathbf{u}$  defines the surface stress vector  $\mathbf{T}$ . Thus  $H = \rho \mathbf{g}$  (here  $\mathbf{g}$  is body force per unit mass) and  $h_n = \mathbf{T}$ .

Accordingly, the conservation law requires the existence of a second rank tensor, the stress tensor  $\boldsymbol{\sigma}$  ( $= \sigma_{ij} \mathbf{e}_i \mathbf{e}_j$ ), satisfying

$$\mathbf{T} = \mathbf{n} \cdot \boldsymbol{\sigma} \quad (T_j = n_i \sigma_{ij})$$

Evidently,  $\sigma_{ij} \mathbf{e}_j$  is the stress vector  $\mathbf{T}$  associated with a surface element having the unit outward normal  $\mathbf{n} = \mathbf{e}_i$  at the point of interest.

Thus, with  $F = \rho \mathbf{u}$ ,  $H = \rho \mathbf{g}$  and  $h_n = \mathbf{n} \cdot \boldsymbol{\sigma}$ , the local form is

$$(\rho \mathbf{u})_{,t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}$$

and simplifying with use of conservation of mass, this becomes

$$\rho (\mathbf{u}_{,t} + \mathbf{u} \cdot \nabla \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} \quad \text{or} \quad \rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}$$

### Angular Momentum:

In this case,  $F = \rho \mathbf{x} \times \mathbf{u}$ ,  $H = \rho \mathbf{x} \times \mathbf{g}$ , and  $h_n = \mathbf{x} \times \mathbf{T} = \mathbf{x} \times (\mathbf{n} \cdot \boldsymbol{\sigma})$  so that the associated 2nd rank tensor  $h$ , associated with the vector  $h_n$  by  $h_n = \mathbf{n} \cdot h$ , is  $h = -\boldsymbol{\sigma} \times \mathbf{x}$ . The local expression is then

$$(\rho \mathbf{x} \times \mathbf{u})_{,t} + \nabla \cdot (\mathbf{u}(\rho \mathbf{x} \times \mathbf{u})) = \nabla \cdot (-\boldsymbol{\sigma} \times \mathbf{x}) + \rho \mathbf{x} \times \mathbf{g}$$

That can be greatly simplified by use of conservation of mass and of linear momentum so that there results an expression which is given most simply in component form as

$$\sigma_{ij} \mathbf{e}_i \times \mathbf{e}_j = 0 \quad (\text{implying that } \sigma_{ij} = \sigma_{ji})$$

That is,  $\boldsymbol{\sigma}$  is symmetric;  $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$ .

### Energy:

Now  $F = \rho (e + \frac{1}{2}|\mathbf{u}|^2)$ , and the energy generation terms are  $H = \rho \mathbf{g} \cdot \mathbf{u} + r$  in the volume, where  $r$  is the rate of radiant energy supply per unit volume, and  $h_n = \mathbf{T} \cdot \mathbf{u} - q_n$  on the surface, where  $q_n$  is the rate of heat outflow per unit area across  $S$ . As before,  $h_n$  can be represented as  $\mathbf{n} \cdot \mathbf{h}$  where in this case, for which  $h_n$  is a scalar,  $\mathbf{h}$  will be a vector. In particular,  $\mathbf{h} = \boldsymbol{\sigma} \cdot \mathbf{u} - \mathbf{q}$  where the heat flow vector  $\mathbf{q}$ , the existence of which is a consequence of the conservation law, satisfies  $q_n = \mathbf{n} \cdot \mathbf{q}$  on  $S$ .

The resulting local form is

$$[\rho (e + \frac{1}{2}|\mathbf{u}|^2)]_{,t} + \nabla \cdot [\rho \mathbf{u} (e + \frac{1}{2}|\mathbf{u}|^2)] = \nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{u}) + \rho \mathbf{g} \cdot \mathbf{u} - \nabla \cdot \mathbf{q} + r$$

and simplifying with the use of conservation of mass and linear and angular momentum, the energy equation is

$$\rho (e_{,t} + \mathbf{u} \cdot \nabla e) = \boldsymbol{\sigma} : \mathbf{D} - \nabla \cdot \mathbf{q} + r \quad \text{or} \quad \rho \frac{De}{Dt} = \boldsymbol{\sigma} : \mathbf{D} - \nabla \cdot \mathbf{q} + r$$

where

$$\mathbf{D} = \text{sym}(\nabla \mathbf{u}) \equiv \frac{1}{2} [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T]$$

is the rate of deformation tensor.

It may be observed that  $\boldsymbol{\sigma} : \mathbf{D}$  ( $= \sigma_{ij} D_{ij}$ ) is the rate of stress working per unit volume, and therefore that  $w$ , the *rate of stress working per unit mass*, is given by

$$w \equiv \frac{\boldsymbol{\sigma} : \mathbf{D}}{\rho}$$

In terms of  $w$ , the last form of the energy equation reads  $De/Dt = w + (r - \nabla \cdot \mathbf{q})/\rho$ , which is the form expected from elementary considerations when it is recognized that  $(r - \nabla \cdot \mathbf{q})/\rho$  is the rate of heat absorption per unit mass.

For example, in the case that the stress state is just a pure hydrostatic pressure  $p$ , i.e. when  $\sigma_{ij} = -p \delta_{ij}$ , like for inviscid fluid models, it is seen that  $\boldsymbol{\sigma} : \mathbf{D} \equiv \sigma_{ij} D_{ij} = -p D_{jj} = -p \nabla \cdot \mathbf{u} = p (D\rho/Dt)/\rho$ , where the last form given above for conservation of mass has been used. Thus  $w = p (D\rho/Dt)/\rho^2 = -p D(1/\rho)/Dt$ , which is the expected result in this case.

**[Aside on elasticity** (not required for ES 220): In the case of elastic materials, energy  $e$  and other thermodynamic functions of state would depend on strain  $\mathbf{E}$  from a reference configuration as well as on another state variable such as temperature or entropy  $s$  per unit mass. Several appropriate definitions of  $\mathbf{E}$  can be made. For example, letting  $\rho_o$  and  $\mathbf{X}$

denote  $\rho$  and  $\mathbf{x}$  in the reference configuration, one commonly adopted definition of  $\mathbf{E}$  is as the *Green strain*  $\mathbf{E}$ , which is based on the change in metric tensor under deformation. It is defined by requiring that  $d\mathbf{x} \cdot d\mathbf{x} = d\mathbf{X} \cdot d\mathbf{X} + 2 d\mathbf{X} \cdot \mathbf{E} \cdot d\mathbf{X}$  for arbitrary choices of  $d\mathbf{X}$ . Here  $d\mathbf{x}$  denotes the material line element which was described by  $d\mathbf{X}$  when in the reference configuration. Thinking of  $\mathbf{x}$  as a function of  $\mathbf{X}$  and  $t$ , and writing  $dx_i = (\partial x_i / \partial X_k) dX_k$  this then defines the components of  $\mathbf{E}$  as

$$E_{kl} = \frac{1}{2} \left( \frac{\partial x_i}{\partial X_k} \frac{\partial x_i}{\partial X_l} - \delta_{kl} \right) = \frac{1}{2} \left( \frac{\partial \xi_k}{\partial X_l} + \frac{\partial \xi_l}{\partial X_k} + \frac{\partial \xi_i}{\partial X_k} \frac{\partial \xi_i}{\partial X_l} \right)$$

where  $\xi = \mathbf{x} - \mathbf{X}$  is the displacement of the considered material particle from its reference position. A work-conjugate symmetric stress tensor  $\mathbf{S}$ , called the *second Piola-Kirchhoff stress*, may then be defined with the property

$$w = \frac{\boldsymbol{\sigma} : \mathbf{D}}{\rho} = \frac{\mathbf{S} : D\mathbf{E}/Dt}{\rho_o} \quad \text{which implies that} \quad \mathbf{S} = \det[\mathbf{F}] \mathbf{F}^{-1} \cdot \boldsymbol{\sigma} \cdot \mathbf{F}^{T-1}$$

Here  $\mathbf{F}$  (not to be confused with use of  $F$  above as a general symbol for density of a conserved quantity) is defined by  $d\mathbf{x} = \mathbf{F} \cdot d\mathbf{X}$ , so that it has components  $F_{ij} = \partial x_i / \partial X_j$ ,  $\mathbf{F}^T$  is its transpose ( $F_{ij}^T = F_{ji}$ ),  $\mathbf{F}^{-1}$  is its inverse ( $d\mathbf{X} = \mathbf{F}^{-1} \cdot d\mathbf{x}$ ), and  $\det[\mathbf{F}]$  ( $= \rho_o / \rho$ ) is its determinant.]

### Entropy:

Entropy is not a conserved quantity and, rather, can only be constrained to be non-decreasing in time (second law of thermodynamics). In this case the general integral and local forms of a conservation law above are replaced by the inequalities

$$\int_V \left( \frac{\partial F}{\partial t} + \nabla \cdot (\mathbf{u}F) \right) dV \geq \int_V H dV + \int_S h_n dS \quad (\text{with } h_n = \mathbf{n} \cdot \mathbf{h})$$

and  $F_{,t} + \nabla \cdot (\mathbf{u}F) \geq \nabla \cdot \mathbf{h} + H$

In these expressions we take  $F = \rho s$ ,  $H = r/T$ , and  $\mathbf{h} = -\mathbf{q}/T$  to form what is called the Clausius-Duhem inequality, of which the local form is

$$(\rho s)_{,t} + \nabla \cdot (\rho \mathbf{u} s) \geq -\nabla \cdot \left( \frac{\mathbf{q}}{T} \right) + \frac{r}{T}$$

and which becomes, after simplification with conservation of mass,

$$\rho (s_{,t} + \mathbf{u} \cdot \nabla s) \geq -\nabla \cdot \left( \frac{\mathbf{q}}{T} \right) + \frac{r}{T} \quad \text{or} \quad \rho \frac{Ds}{Dt} \geq \frac{\mathbf{q} \cdot \nabla T}{T^2} - \frac{\nabla \cdot \mathbf{q}}{T} + \frac{r}{T}$$

The last expression can be combined with the energy equation to rewrite the Clausius-Duhem inequality as

$$\frac{De}{Dt} + \frac{\mathbf{q} \cdot \nabla T}{\rho T} \leq \frac{\boldsymbol{\sigma} : \mathbf{D}}{\rho} + T \frac{Ds}{Dt}$$

## Thermodynamic Constraints on Constitutive Laws, Simple Viscous Fluids

For simple viscous fluids, which we think of as compressible in general, we assume that the stress tensor  $\boldsymbol{\sigma}$  is a function of  $\rho$ ,  $T$  and the instantaneous rate of deformation tensor  $\mathbf{D}$  (but not of its history, like would be the case for *complex* fluids).

When  $\mathbf{D} = \mathbf{0}$ ,  $\boldsymbol{\sigma}$  must reduce to its equilibrium value  $\boldsymbol{\sigma}^{eq}$  where  $\sigma_{ij}^{eq} = -p(\rho, T)\delta_{ij}$ . Here  $p(\rho, T)$  is the equilibrium pressure given by the thermal equation of state.

Then when  $\mathbf{D} \neq \mathbf{0}$ , we write

$$\sigma_{ij} = \tau_{ij} + \sigma_{ij}^{eq} \equiv \tau_{ij} - p(\rho, T)\delta_{ij}$$

where  $p(\rho, T)$  continues to be given by the thermal equation of state and the tensor  $\boldsymbol{\tau}$  may be called the *viscous* part of the stress tensor  $\boldsymbol{\sigma}$ .

Other thermodynamic properties such as  $e$  and  $s$  relate to  $\rho$ ,  $T$  and  $p$  just like at equilibrium, i.e., in a manner constrained by continuing validity of the perfect differential form

$$-p d(1/\rho) + T ds = de ,$$

that is, of

$$-p \frac{D(1/\rho)}{Dt} + T \frac{Ds}{Dt} = \frac{De}{Dt} .$$

We now observe that because  $D_{kk} = (D(1/\rho)/Dt)/(1/\rho)$ ,

$$-p \frac{D(1/\rho)}{Dt} = -\frac{pD_{kk}}{\rho} \equiv \frac{\sigma^{eq} : \mathbf{D}}{\rho} \equiv \frac{(\boldsymbol{\sigma} - \boldsymbol{\tau}) : \mathbf{D}}{\rho}$$

and the equation before this last one then becomes an expression for  $De/Dt$  in the form

$$\frac{De}{Dt} = T \frac{Ds}{Dt} + \frac{(\boldsymbol{\sigma} - \boldsymbol{\tau}) : \mathbf{D}}{\rho}$$

Substituting this last expression into the thermodynamic inequality given just before the start of this section, and cancelling like terms on each side, we get (after multiplying through by  $-\rho$ )

$$\boldsymbol{\tau} : \mathbf{D} - \mathbf{q} \cdot (\boldsymbol{\nabla}T)/T \geq 0 .$$

This must hold for all possible  $\mathbf{D}$  and  $\boldsymbol{\nabla}T$ , and for all  $\rho$  and  $T$ .

Now, by our assumptions about the viscous stress,  $\boldsymbol{\tau}$  is a function only of  $\rho$ ,  $T$  and  $\mathbf{D}$ , but not of  $\boldsymbol{\nabla}T$ . Thus, the inequality still gives a valid general constraint at points in space-time for which  $\boldsymbol{\nabla}T = \mathbf{0}$ , and such points could in principle be encountered for any values of  $\rho$ ,  $T$  and  $\mathbf{D}$ . Hence we must require that

$$\boldsymbol{\tau} : \mathbf{D} \geq 0$$



for all  $\rho$ ,  $T$  and  $\mathbf{D}$ . In a related manner, when  $\mathbf{D} = \mathbf{0}$  it is clear that the inequality

$$-\mathbf{q} \cdot \nabla T \geq 0$$

It must hold for *all*  $\mathbf{D}$ , assuming that  $\mathbf{q}$  is a function only of  $\rho$ ,  $T$  and  $\nabla T$ , but not  $\mathbf{D}$ .

**Linear viscous resistance and heat conduction relations:** We here make the conventional additional assumptions that  $\boldsymbol{\tau}$  is linear in  $\mathbf{D}$ , and that  $\mathbf{q}$  is linear in  $\nabla T$ , in ways that recognize the isotropy of fluid properties. The most general\* laws of that type are

$$\boldsymbol{\tau}' = 2\mu\mathbf{D}' \quad \text{and} \quad \text{tr}(\boldsymbol{\tau})/3 = \kappa \text{tr}(\mathbf{D}) \quad (\text{Newtonian viscosity})$$

[where  $\boldsymbol{\tau}' \equiv \boldsymbol{\tau} - \text{tr}(\boldsymbol{\tau})\mathbf{I}/3$  and  $\text{tr}(\boldsymbol{\tau}) \equiv \tau_{kk}$ ; similarly  $\mathbf{D}' \equiv \mathbf{D} - \text{tr}(\mathbf{D})\mathbf{I}/3$  and  $\text{tr}(\mathbf{D}) \equiv D_{kk}$ ; here “tr” stands for “trace”, or sum of diagonal elements] and

$$\mathbf{q} = -K\nabla T \quad (\text{Fourier law for heat conduction}),$$

The factors in those equations are the *shear viscosity*  $\mu$ , the *bulk viscosity*  $\kappa$ , and the *thermal conductivity*  $K$ . In general, all are functions of  $\rho$  and  $T$ .

The “primed” quantities  $\boldsymbol{\tau}'$ ,  $\mathbf{D}'$ , and  $\boldsymbol{\sigma}'$  are called the *deviatoric parts* of  $\boldsymbol{\tau}$ ,  $\mathbf{D}$  and  $\boldsymbol{\sigma}$ , respectively, and we note that  $\text{tr}(\boldsymbol{\tau}') = 0$ ,  $\text{tr}(\mathbf{D}') = 0$  and  $\text{tr}(\boldsymbol{\sigma}') = 0$ . Also, the relation  $\boldsymbol{\sigma} = \boldsymbol{\tau} - p\mathbf{I}$  shows that the stress tensor satisfies

$$\boldsymbol{\sigma}' \equiv \boldsymbol{\tau}' = 2\mu\mathbf{D}' \quad \text{and} \quad \text{tr}(\boldsymbol{\sigma})/3 \equiv \text{tr}(\boldsymbol{\tau})/3 - p = \kappa \text{tr}(\mathbf{D}) - p.$$

That may be rewritten as an equivalent single expression for  $\boldsymbol{\sigma}$  (rather than separately for its deviatoric part and its trace) as

$$\boldsymbol{\sigma} = \boldsymbol{\tau} - p\mathbf{I} = 2\mu\mathbf{D} + (\kappa - 2\mu/3)\text{tr}(\mathbf{D})\mathbf{I} - p\mathbf{I},$$

and the expressions may be inverted to represent  $\mathbf{D}$  as

$$\mathbf{D} = \frac{1}{2\mu}\boldsymbol{\tau} - \left(\frac{1}{6\mu} - \frac{1}{9\kappa}\right)\text{tr}(\boldsymbol{\tau})\mathbf{I} = \frac{1}{2\mu}\boldsymbol{\sigma} - \left(\frac{1}{6\mu} - \frac{1}{9\kappa}\right)\text{tr}(\boldsymbol{\sigma})\mathbf{I} + \frac{1}{3\kappa}p\mathbf{I}.$$

In these equations, we recall that  $p$  is the function  $p = p(\rho, T)$  characterizing the thermal equation of state, and is *not* to be equated to  $-\text{tr}(\boldsymbol{\sigma})/3$  (unless  $\kappa = 0$  and/or  $\text{tr}(\mathbf{D}) = 0$ ). For example, if an “isotropic” stress state  $\sigma_{11} = \sigma_{22} = \sigma_{33} = -C$  (the notation  $C$  is used to denote a *compressive* stress), with off-diagonal  $\sigma_{ij} = 0$ , is applied to a fluid element, the corresponding deformation rates will satisfy  $D_{11} = D_{22} = D_{33}$ , and off-diagonal  $D_{ij} = 0$ , where  $3\kappa D_{11} = p(\rho, T) - C$ . Recognizing that  $3D_{11} = -(1/\rho)D\rho/Dt$  in this circumstance, it is seen that  $\rho$  would evolve according to the first order differential equation  $\kappa D\rho/Dt = \rho[C - p(\rho, T)]$ . To characterize the solution to that differential equation, we would have to say something about the thermal conditions on the fluid element. In the simplest case, when

we assume  $T$  is held fixed by appropriate heat extraction from the element, it is easy to see that for fixed  $C$ ,  $\rho$  will evolve monotonically, at a finite rate, towards the value which makes  $p(\rho, T) = C$ , provided that  $\kappa > 0$  (see next sub-section) and that the isothermal compressibility is positive (assured by  $\partial p(\rho, T)/\partial \rho > 0$ ).

[\* At the start of this sub-section expressions were given for  $\boldsymbol{\tau}'$ ,  $\text{tr}(\boldsymbol{\tau})$  and  $\mathbf{q}$  (or, equivalently, for  $\boldsymbol{\tau}$  and  $\mathbf{q}$ ) which were claimed to provide the most general possible linear relations to  $\mathbf{D}$  and  $\nabla T$  for an isotropic material. It is easy to understand that the result stated for  $\mathbf{q}$  satisfies that claim, but the relation given between  $\boldsymbol{\tau}$  and  $\mathbf{D}$  may merit more discussion. Such is provided here, making use of the symmetry of  $\boldsymbol{\tau}$  (which holds because of symmetry of  $\boldsymbol{\sigma}$  and  $\mathbf{I}$ ). That symmetry means that at any given  $\mathbf{x}$  and  $t$ , there exist three mutually orthogonal *principal* directions so that  $\boldsymbol{\tau}$  is diagonal relative to those axes. Let those directions be chosen as the 1, 2 and 3 directions, so that the  $\tau_{ij}$  vanish if  $i \neq j$ . Now we make use of *linearity* and *isotropy*. By *linearity* the instantaneous response  $\mathbf{D}$  to  $\boldsymbol{\tau}$  is the sum of the separate responses to  $\tau_{11}, \tau_{22}$  and  $\tau_{33}$ . By *isotropy* the response to  $\tau_{11}$  alone must be of the form

$$D_{11} = A \tau_{11}, \quad D_{22} = D_{33} = -B \tau_{11}, \quad D_{ij} = 0 \text{ for } i \neq j$$

where  $A$  and  $B$  are scalar fluid properties. The response to  $\tau_{22}$  alone, and to  $\tau_{33}$  alone, may be written similarly, changing 1,2,3 to 2,3,1, and to 3,1,2, respectively, keeping the same factors  $A$  and  $B$ . Thus, summing these separate linear responses, we conclude that, e.g.,

$$D_{11} = A \tau_{11} - B \tau_{22} - B \tau_{33} = (A + B) \tau_{11} - B (\tau_{11} + \tau_{22} + \tau_{33})$$

with similar expressions for  $D_{22}$  and  $D_{33}$ , and with the off-diagonal  $D_{ij} = 0$ . Thus, in this special, local principal axes coordinate system,

$$D_{ij} = (A + B) \tau_{ij} - B \delta_{ij} \tau_{kk}$$

holds for all  $i, j$ , i.e., for all deformation and stress components. However,  $D_{ij}$ ,  $\tau_{ij}$  and  $\delta_{ij}$  are second rank tensors, whereas  $\tau_{kk}$  is invariant under coordinate transformation. Thus if we choose any other orthogonal coordinate directions which are rotated from the principal axes, the same relation between components of  $\mathbf{D}$  and  $\boldsymbol{\tau}$  must hold in that new system. Renaming  $A$  and  $B$  in terms of  $\mu$  and  $\kappa$ , that justifies the form asserted for relations between  $\mathbf{D}$  and  $\boldsymbol{\tau}$  towards the start of this sub-section.]

**Requirement of non-negative viscosities and conductivity:** It is easy to show that the viscous dissipation rate  $\boldsymbol{\tau} : \mathbf{D}$  satisfies

$$\boldsymbol{\tau} : \mathbf{D} = \boldsymbol{\tau}' : \mathbf{D}' + \text{tr}(\boldsymbol{\tau}) \text{tr}(\mathbf{D})/3 = 2\mu (\mathbf{D}' : \mathbf{D}') + \kappa [\text{tr}(\mathbf{D})]^2.$$

Thus the thermodynamic inequality  $\boldsymbol{\tau} : \mathbf{D} - \mathbf{q} \cdot (\nabla T)/T \geq 0$  becomes

$$2\mu (\mathbf{D}' : \mathbf{D}') + \kappa [\text{tr}(\mathbf{D})]^2 + K |\nabla T|^2/T \geq 0.$$

That can be satisfied for all possible  $\mathbf{D}$  [meaning all possible  $\mathbf{D}'$  and  $\text{tr}(\mathbf{D})$ ] and  $\nabla T$  as may arise in flow processes only if all of  $\mu$ ,  $\kappa$  and  $K$  are *non-negative*.

## Energy Equation

We now recall the energy conservation equation  $\rho De/Dt = \boldsymbol{\sigma} : \mathbf{D} - \nabla \cdot \mathbf{q} + r$  as well as the above transformation of the thermodynamic identity  $-p d(1/\rho) + T ds = de$  into  $\rho De/Dt = \rho T Ds/Dt + (\boldsymbol{\sigma} - \boldsymbol{\tau}) : \mathbf{D}$ . Eliminating  $De/Dt$  from the expressions, and using  $\mathbf{q} = -K\nabla T$ , allows the energy equation to be rewritten as

$$\nabla \cdot (K \nabla T) + \boldsymbol{\tau} : \mathbf{D} + r = \rho T \frac{Ds}{Dt}$$

In this expression, we recall that  $s$  is related to  $p$ ,  $\rho$  and  $T$  (themselves related by  $p = p(\rho, T)$ ) just as for equilibrium states. Thus we may write  $s = s(T, \rho)$  or  $s = s(T, p)$ , according to preference, and write

$$\frac{Ds}{Dt} = \frac{\partial s(T, \rho)}{\partial T} \frac{DT}{Dt} + \frac{\partial s(T, \rho)}{\partial \rho} \frac{D\rho}{Dt} \quad \text{or} \quad \frac{Ds}{Dt} = \frac{\partial s(T, p)}{\partial T} \frac{DT}{Dt} + \frac{\partial s(T, p)}{\partial p} \frac{Dp}{Dt},$$

Two of the above partial derivatives of  $s$  are given in terms of specific heats per unit mass,  $c_v$  or  $c_p$ , at constant  $\rho$  or  $p$ , respectively, as  $\partial s(T, \rho)/\partial T = c_v/T$  and  $\partial s(T, p)/\partial T = c_p/T$ . Maxwell reciprocal relations associated with recognition that  $-p d(1/\rho) - s dT$  and  $dp/\rho - s dT$  are perfect differentials enable the other partial derivatives to be computed from the thermal equation of state.

The result may be written as

$$\nabla \cdot (K \nabla T) + \boldsymbol{\tau} : \mathbf{D} + r = \rho c_v \frac{DT}{Dt} - \hat{\beta} \frac{p}{\rho} \frac{D\rho}{Dt},$$

$$\text{or as} \quad \nabla \cdot (K \nabla T) + \boldsymbol{\tau} : \mathbf{D} + r = \rho c_p \frac{DT}{Dt} - \hat{\alpha} \frac{Dp}{Dt},$$

$$\text{where} \quad \hat{\beta} = \frac{T}{p} \frac{\partial p(\rho, T)}{\partial T} \quad \text{and} \quad \hat{\alpha} = -\frac{T}{\rho} \frac{\partial \rho(p, T)}{\partial T}.$$

It may be noted that  $\hat{\alpha} > 0$  when the thermal expansion under fixed pressure is positive, and then  $\hat{\beta} > 0$  too, so long as  $p > 0$  and the isothermal compressibility of the fluid is positive (as we would always assume on grounds of thermodynamic stability). Also, for an ideal gas,  $\hat{\beta} = \hat{\alpha} = 1$ .

**Simplified energy equation:** In simplified analyses of some flow and heat transfer problems, distinctions between  $c_v$  and  $c_p$  are ignored (with notation  $c$  used instead), and the

$D\rho/Dt$  and  $Dp/Dt$  terms are ignored (they are often small compared to other terms), so that the energy equation is written approximately as

$$\nabla \cdot (K \nabla T) + \boldsymbol{\tau} : \mathbf{D} + r = \rho c \frac{DT}{Dt}.$$