## **Differential Balances - Alternate Forms**

To recall, differential balance equations express the basic laws of conservation of mass, momentum, and energy:

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\nabla\cdot\mathbf{v} \qquad (\text{conservation of mass}) \tag{1}$$

$$\rho \frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t} = \mathbf{B} + \nabla \cdot \boldsymbol{\sigma} \qquad (\text{momentum balance}) \tag{2}$$

$$\rho \frac{\mathrm{D}e}{\mathrm{D}t} = -\nabla \cdot \mathbf{q} + q^{\prime \prime \prime} + \nabla \cdot (\mathbf{\sigma} \cdot \mathbf{v}) \qquad (\text{conservation of energy}) \tag{3}$$

Here, the operator D/Dt is the "material derivative" and is defined by

$$\frac{\mathbf{D}}{\mathbf{D}t} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$$

Below we consider how these expressions are modified when applied to certain common types of fluid flows.

**1. Equation of Continuity (conservation of mass).** Beside the full equation (1), the only other version important for this course is for an incompressible fluid, for which

$$\nabla \cdot \mathbf{v} = 0 \qquad (\text{incompressible fluid}) \tag{4}$$

Equation (4) has already been encountered earlier.

### 2. Equation of Change of Momentum (momentum balance).

**2.1). Euler Equations.** Perhaps the simplest type of fluid is one for which no viscous stresses exist. For such a "frictionless" flow, the stress tensor  $\sigma$  in equation (2) is simply

$$\sigma_{ij} = -p\,\delta_{ij} \tag{5}$$

where p is the (thermodynamic) pressure in the fluid (Aside: note that in ideal flow the mechanical and thermodynamic pressures are equal). Equation 5 states that since there are no viscous stresses in a frictionless flow, the only kind of stress present is the normal, compressive stress due to pressure. The

*j*th component of 
$$\nabla \cdot \boldsymbol{\sigma}$$
 is  $\frac{\partial \sigma_{ij}}{\partial x_i}$ , and using equation (5) this becomes  $-\frac{\partial p \,\delta_{ij}}{\partial x_i} = -\delta_{ij} \frac{\partial p}{\partial x_i} =$ 

 $-\frac{\partial p}{\partial x_j}$ . Therefore, the *j*th component of equation (2) is

$$\rho \frac{\mathrm{D}v_j}{\mathrm{D}t} = B_j - \frac{\partial p}{\partial x_j} \tag{6}$$

Written out in full for the  $x_1$  component in the CCS system, equation (6) is

$$\rho \left( \frac{\partial v_1}{\partial t} + v_1 \frac{\partial v_1}{\partial x_1} + v_2 \frac{\partial v_1}{\partial x_2} + v_3 \frac{\partial v_1}{\partial x_3} \right) = B_1 - \frac{\partial p}{\partial x_1}$$
(7)

with analogous expressions for the  $x_2$  and  $x_3$  components (you should be able to readily write these out). Equation (7) and its  $x_2$  and  $x_3$  forms are known as the Euler Equations.

When viewed in terms of the material derivative notation, equation (6) states that, for a frictionless fluid, the rate of change of *j*-direction momentum of a fluid element moving with the flow (left hand side) equals the *j*-direction body force (first term on the right) plus the *j*-direction pressure force (second term on the right) acting on the fluid element.

*Recall*: For a fluid element moving with the flow, the boundaries of the fluid element move with the bulk velocity  $\mathbf{v}$  so that no convective transfer of any quantity (mass, momentum, or energy) occurs across the surface of the fluid element; therefore, momentum of a fluid element moving with the flow can only be altered by forces exerted on the fluid element.

When using the Euler equations to describe fluid flow, it is assumed that friction between different parts of the fluid that move relative to each other is negligible. It is important to realize that this does not necessarily imply the assumption of a viscosity  $\mu$  that is close to zero. For example, it is possible that the velocity gradients in the fluid are simply so small so that the relative motion between neighboring parts of the fluid is very slight, and the friction generated is thus negligible even though the viscosity may be significant.

**2.2).** Navier-Stokes Equations. The Navier-Stokes equations are the differential momentum balance written for a Newtonian fluid. The differential momentum balance is given by equation (2) above. To specialize it to a Newtonian fluid, the Newtonian expression (i.e. the "constitutive relation") for the stress tensor  $\sigma$  must be substituted into equation (2). The stress tensor for a Newtonian fluid is given by (note that here, and throughout this handout, *p* is the thermodynamic pressure)

$$\sigma_{ij} = -p \delta_{ij} + \lambda \left( \nabla \bullet \mathbf{v} \right) \, \delta_{ij} + 2\mu \, e_{ij} \tag{8}$$

We recall that the *off-diagonal*, i.e.  $i \neq j$ , components of  $e_{ij}$  are proportional to rate of shear strain, while the diagonal components of  $e_{ij}$ , i = j, are related to the rate of dilatational strain. In Cartesian notation, equation 8 becomes

$$\sigma_{ij} = -p\delta_{ij} + \lambda \left(\frac{\partial v_k}{\partial x_k}\right) \delta_{ij} + \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)$$
(9)

The momentum balance requires an expression for  $\nabla \cdot \boldsymbol{\sigma}$ . The *j*th component of  $\nabla \cdot \boldsymbol{\sigma}$  is  $\frac{\partial \sigma_{ij}}{\partial x_i}$ ;

therefore, using equation 9,

$$(\nabla \cdot \boldsymbol{\sigma})_{j} = -\frac{\partial p \,\delta_{ij}}{\partial x_{i}} + \frac{\partial}{\partial x_{i}} \left[\lambda \left(\frac{\partial v_{k}}{\partial x_{k}}\right) \,\delta_{j}\right] + \frac{\partial}{\partial x_{i}} \left[\mu \left(\frac{\partial v_{i}}{\partial x_{j}} + \frac{\partial v_{j}}{\partial x_{i}}\right)\right] = -\frac{\partial p}{\partial x_{j}} + \frac{\partial}{\partial x_{j}} \left[\lambda \left(\frac{\partial v_{k}}{\partial x_{k}}\right)\right] + \frac{\partial}{\partial x_{i}} \left[\mu \left(\frac{\partial v_{i}}{\partial x_{j}} + \frac{\partial v_{j}}{\partial x_{i}}\right)\right]$$
(10)

The Kronecker deltas were summed over in arriving at the last line of equation 10. Substituting equation 10 into the momentum balance equation 2, we obtain the *j*th component of the **Navier-Stokes** equations

$$\rho \frac{\mathrm{D}v_j}{\mathrm{D}t} = B_j - \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j} \left[\lambda \left(\frac{\partial v_k}{\partial x_k}\right)\right] + \frac{\partial}{\partial x_i} \left[\mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right]$$
(11)

The Navier-Stokes equations are the momentum balance expressed for a Newtonian fluid. Setting j = 1 in equation 11 produces the  $x_1$  component momentum balance:

$$\rho \left( \frac{\partial v_1}{\partial t} + v_1 \frac{\partial v_1}{\partial x_1} + v_2 \frac{\partial v_1}{\partial x_2} + v_3 \frac{\partial v_1}{\partial x_3} \right) = B_1 - \frac{\partial p}{\partial x_1} + \frac{\partial}{\partial x_1} \left[ \lambda \left( \frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \frac{\partial v_3}{\partial x_3} \right) \right] \\
+ \frac{\partial}{\partial x_1} \left[ 2\mu \frac{\partial v_1}{\partial x_1} \right] + \frac{\partial}{\partial x_2} \left[ \mu \left( \frac{\partial v_2}{\partial x_1} + \frac{\partial v_1}{\partial x_2} \right) \right] + \frac{\partial}{\partial x_3} \left[ \mu \left( \frac{\partial v_3}{\partial x_1} + \frac{\partial v_1}{\partial x_3} \right) \right] \quad (12)$$

Equation 12 may look formidable compared to the original momentum balance equation 2. However, all we did was substitute in the constitutive relation for a Newtonian fluid, according to equation 9.

For an *incompressible* fluid,  $\nabla \cdot \mathbf{v} = \frac{\partial v_i}{\partial x_i} = 0$ . Moreover, if we also assume a *constant viscosity*  $\mu$  then

equation 11 simplifies to

$$\rho \frac{\mathrm{D}v_{j}}{\mathrm{D}t} = B_{j} - \frac{\partial p}{\partial x_{j}} + \mu \left(\frac{\partial^{2} v_{i}}{\partial x_{i} \partial x_{j}} + \frac{\partial}{\partial x_{i}} \frac{\partial v_{j}}{\partial x_{i}}\right)$$

Since  $\frac{\partial^2 v_i}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\partial v_i}{\partial x_i} \right) = 0$  due to incompressibility,

$$\rho \frac{\mathrm{D}v_{j}}{\mathrm{D}t} = B_{j} - \frac{\partial p}{\partial x_{j}} + \mu \frac{\partial}{\partial x_{i}} \frac{\partial v_{j}}{\partial x_{i}}$$
(13)

Equation 13 holds for incompressible, constant viscosity Newtonian fluids and is one of the most frequently used forms of the differential momentum balance. Along the three directions  $x_1$ ,  $x_2$ , and  $x_3$  (corresponding to j = 1, 2, and 3), equation 13 is

$$\rho\left(\frac{\partial v_1}{\partial t} + v_1\frac{\partial v_1}{\partial x_1} + v_2\frac{\partial v_1}{\partial x_2} + v_3\frac{\partial v_1}{\partial x_3}\right) = B_1 - \frac{\partial p}{\partial x_1} + \mu\left(\frac{\partial^2 v_1}{\partial x_1^2} + \frac{\partial^2 v_1}{\partial x_2^2} + \frac{\partial^2 v_1}{\partial x_3^2}\right)$$
(14a)

$$\rho\left(\frac{\partial v_2}{\partial t} + v_1\frac{\partial v_2}{\partial x_1} + v_2\frac{\partial v_2}{\partial x_2} + v_3\frac{\partial v_2}{\partial x_3}\right) = B_2 - \frac{\partial p}{\partial x_2} + \mu\left(\frac{\partial^2 v_2}{\partial x_1^2} + \frac{\partial^2 v_2}{\partial x_2^2} + \frac{\partial^2 v_2}{\partial x_3^2}\right) \quad (14b)$$

$$\rho\left(\frac{\partial v_3}{\partial t} + v_1\frac{\partial v_3}{\partial x_1} + v_2\frac{\partial v_3}{\partial x_2} + v_3\frac{\partial v_3}{\partial x_3}\right) = B_3 - \frac{\partial p}{\partial x_3} + \mu\left(\frac{\partial^2 v_3}{\partial x_1^2} + \frac{\partial^2 v_3}{\partial x_2^2} + \frac{\partial^2 v_3}{\partial x_3^2}\right)$$
(14c)

Equations 14 can be summarized much more compactly in tensor notation as

$$\rho \frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t} = \mathbf{B} - \nabla p + \mu \nabla^2 \mathbf{v} \qquad \text{(incompressible, constant } \mu \text{ Newtonian fluids)} \tag{15}$$

When coordinate systems other than CCS are used, equation 15 will not need to be rederived since the basic law of momentum conservation that it represents must remain valid. However, to express equation 15 in another coordinate system, the forms for the operators D/Dt,  $\nabla$  and  $\nabla^2$  appropriate to

that coordinate system must be used. Equation 15 states that for a fluid element moving with an incompressible, constant viscosity Newtonian flow, the rate of change of momentum (left hand side) equals the sum of the body force (first term on right), pressure force (second term on right), and viscous force (third term on right) that act on the fluid element.

### 3. Conservation of Energy

The differential law of energy conservation, equation 3, is

$$\rho \frac{\mathrm{D}e}{\mathrm{D}t} = -\nabla \cdot \mathbf{q} + q^{'''} + \nabla \cdot (\mathbf{\sigma} \cdot \mathbf{v}) \tag{16}$$

To specialize equation 16 to a Newtonian fluid, equation 9 for the stress tensor  $\boldsymbol{\sigma}$  needs to be substituted into the term  $\nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{v})$ . We will do just that after rearranging 16 into a more useful form. We note that, using the definition of the inner product for tensors, in Cartesian notation the term  $\nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{v})$  becomes (can you show this?)

$$\nabla \bullet (\mathbf{\sigma} \bullet \mathbf{v}) = \partial/\partial x_i \left( \sigma_{ij} v_j \right) \tag{17}$$

## **3.1). Mechanical Energy Balance.**

The Mechanical Energy Equation is concerned with kinetic and potential energies only. The internal energy is not included. Therefore, this equation will *not* represent the law of energy conservation, since it is not a total energy balance. The Mechanical Energy Equation can be derived directly from the rate of change of momentum equation, equation 2, which if expanded in CCS reads (you should be able to perform this expansion on your own)

$$\rho \frac{\mathrm{D}v_1}{\mathrm{D}t} \boldsymbol{\delta}_1 + \rho \frac{\mathrm{D}v_2}{\mathrm{D}t} \boldsymbol{\delta}_2 + \rho \frac{\mathrm{D}v_3}{\mathrm{D}t} \boldsymbol{\delta}_3 = \rho g_1 \boldsymbol{\delta}_1 + \rho g_2 \boldsymbol{\delta}_2 + \rho g_3 \boldsymbol{\delta}_3 + (\frac{\partial \sigma_{11}}{\partial x_1} + \frac{\partial \sigma_{21}}{\partial x_2} + \frac{\partial \sigma_{31}}{\partial x_3}) \boldsymbol{\delta}_1 + (\frac{\partial \sigma_{12}}{\partial x_1} + \frac{\partial \sigma_{22}}{\partial x_2} + \frac{\partial \sigma_{32}}{\partial x_3}) \boldsymbol{\delta}_2 + (\frac{\partial \sigma_{13}}{\partial x_1} + \frac{\partial \sigma_{23}}{\partial x_2} + \frac{\partial \sigma_{33}}{\partial x_3}) \boldsymbol{\delta}_3$$
(18)

Or, in tensor notation,

$$\rho \frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t} = \rho \mathbf{g} + \nabla \cdot \boldsymbol{\sigma} \tag{19}$$

For definiteness, we took the body force per unit volume **B** to be equal to the gravitational force,  $\mathbf{B} = \rho$ **g**. Taking the dot product of equation (19) with the velocity **v** results in

$$\rho \mathbf{v} \cdot \frac{\mathbf{D} \mathbf{v}}{\mathbf{D} t} = \mathbf{v} \cdot (\rho \mathbf{g} + \nabla \cdot \boldsymbol{\sigma}) \tag{20}$$

We could prove that

$$\rho \mathbf{v} \cdot \frac{\mathbf{D}\mathbf{v}}{\mathbf{D}t} = \frac{\rho}{2} \frac{\mathbf{D}(\mathbf{v} \cdot \mathbf{v})}{\mathbf{D}t} = \rho \frac{\mathbf{D}(v^2/2)}{\mathbf{D}t}$$
(21)

Using equation 21, equation 20 becomes

$$\rho \frac{\mathrm{D}(v^2/2)}{\mathrm{D}t} = \rho \,\mathbf{v} \cdot \mathbf{g} + \mathbf{v} \cdot (\nabla \cdot \boldsymbol{\sigma}) \tag{22}$$

Now we make use of some facts: (i)  $g_z$ , the gravitational potential per unit mass at a point at height z, does not change with time so that  $\partial(gz)/\partial t = 0$ , and (ii) if the gravitational acceleration g is constant, then the gravitational force per unit mass  $\mathbf{g} = -g\mathbf{n}_Z = -g\nabla z = -\nabla(gz)$ . Here,  $\mathbf{n}_Z = \nabla z$  is a unit vector pointing in the positive z direction. Adding  $\rho \partial(gz)/\partial t$  to the left hand side and substituting -  $\nabla(gz)$  for g, equation 22 rearranges to

$$\rho \frac{\mathrm{D}(v^2/2)}{\mathrm{D}t} + \rho \{ \frac{\partial(gz)}{\partial t} + \mathbf{v} \cdot \nabla(gz) \} = \mathbf{v} \cdot (\nabla \cdot \mathbf{\sigma})$$

Note that it was allowable to add  $\rho \partial (gz)/\partial t$  only to the left hand side since this term equals 0. Using the definition of the material derivative,  $\frac{\partial(gz)}{\partial t} + \mathbf{v} \cdot \nabla(gz) = D(gz)/Dt$ , and the above expression

rearranges to

$$\rho \frac{\mathrm{D}(v^2/2 + gz)}{\mathrm{D}t} = \mathbf{v} \cdot (\nabla \cdot \boldsymbol{\sigma})$$
(23)

Equation 23 is called the **Mechanical Energy Equation**. The term "mechanical" is meant to emphasize that the equation is only concerned with kinetic and gravitational potential energies and does not include the internal energy. That equation 23 is only a balance on kinetic and gravitational potential energies is evident from its left hand side. We will next use equation 23 to derive a differential balance on internal energy.

**3.2). Differential Balance on Internal Energy.** A balance on internal energy is obtained by subtracting the balance on mechanical (kinetic + potential) energy (equation 23) from the balance on total (internal + kinetic + potential) energy (equation 16). We have

$$\rho \frac{De}{Dt} = -\nabla \cdot \mathbf{q} + q''' + \nabla \cdot (\mathbf{\sigma} \cdot \mathbf{v}) \qquad (\text{total energy balance})$$
$$\rho \frac{D(v^2/2 + gz)}{Dt} = \mathbf{v} \cdot (\nabla \cdot \mathbf{\sigma}) \qquad (\text{mechanical energy balance})$$

Recalling that  $e = u + v^2/2 + gz$ , subtraction of the mechanical energy equation from the total energy balance leads to

$$\rho \frac{\mathcal{D}(u+v^2/2+gz-v^2/2-gz)}{\mathcal{D}t} = -\nabla \cdot \mathbf{q} + q^{'''} + \nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{v}) - \mathbf{v} \cdot (\nabla \cdot \boldsymbol{\sigma})$$
(24)

or

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = -\nabla \cdot \mathbf{q} + q^{'''} + \nabla \cdot (\boldsymbol{\sigma} \cdot \mathbf{v}) - \mathbf{v} \cdot (\nabla \cdot \boldsymbol{\sigma})$$
(25)

Equation 25 has not referred to any particular coordinate system as yet. However, for the rest of the derivation we will make use of Cartesian coordinates. This is not necessary, but will be a bit easier to follow than staying in the general vector notation.

We recall that the divergence of a vector A is

$$\nabla \cdot \mathbf{A} = \frac{\partial A_i}{\partial x_i} \tag{26}$$

Second, from equation 17

$$\nabla \cdot (\mathbf{\sigma} \cdot \mathbf{v}) = \frac{\partial (\sigma_{ij} v_j)}{\partial x_i}$$
(27)

Third, by procedures similar to those used to derive equation (27), we could show that

$$\mathbf{v} \bullet (\nabla \bullet \mathbf{\sigma}) = v_j \frac{\partial \sigma_{ij}}{\partial x_i}$$
(28)

Using equations 26, 27, and 28, equation 25 rearranges to

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = -\frac{\partial q_i}{\partial x_i} + q''' + \frac{\partial (\sigma_{ij} v_j)}{\partial x_i} - v_j \frac{\partial \sigma_{ij}}{\partial x_i}$$
(29)

According to the product rule of differentiation  $\frac{\partial(\sigma_{ij}v_j)}{\partial x_i} = \sigma_{ij}\frac{\partial v_j}{\partial x_i} + v_j\frac{\partial \sigma_{ij}}{\partial x_i}$ , thus

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = -\frac{\partial q_i}{\partial x_i} + q''' + \sigma_{ij} \frac{\partial v_j}{\partial x_i}$$
(30)

The heat flux vector  $\mathbf{q}$  can be separated into heat flux by conduction  $\mathbf{q}_{\rm C}$ , which obeys Fourier's Law  $\mathbf{q}_{\rm C} = -\kappa \nabla T$ , and heat flux by radiation  $\mathbf{q}_{\rm r}$ . With these modifications the internal energy balance becomes

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = -\frac{\partial q_{Ci}}{\partial x_i} - \frac{\partial q_{ri}}{\partial x_i} + q''' + \sigma_{ij} \frac{\partial v_j}{\partial x_i}$$
(31)

We will now specialize equation 31 to Newtonian fluids that also follow Fourier's Law,  $q_{Ci} = -k \frac{\partial T}{\partial x_i}$  (i.e. we are now specializing to flows of Newtonian fluids that obey Fourier's Law):

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) - \frac{\partial q_{ri}}{\partial x_i} + q''' + \left[ \left\{ -p \delta_{ij} + \lambda \left( \frac{\partial v_k}{\partial x_k} \right) \delta_{ij} + \mu \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \right\} \frac{\partial v_j}{\partial x_i} \right]$$
(32)

The last term on the right (the term inside the [] parentheses) becomes

$$-p\frac{\partial v_j}{\partial x_i}\delta_{j} + \lambda\left(\frac{\partial v_k}{\partial x_k}\right)\frac{\partial v_j}{\partial x_i}\delta_{j} + \mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\frac{\partial v_j}{\partial x_i}$$

Summing over j in the two terms involving the Kronecker delta results in (recall that the Kronecker delta  $\delta_{ij}$  equals zero unless i = j):

$$-p\frac{\partial v_i}{\partial x_i} + \lambda \left(\frac{\partial v_k}{\partial x_k}\right) \frac{\partial v_i}{\partial x_i} + \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) \frac{\partial v_j}{\partial x_i}$$
(33)

Using expression 26 for the divergence of a vector, we see that the *p* in equation 33 is multiplied by  $(\nabla \cdot \mathbf{v})$  and the  $\lambda$  is multiplied by  $(\nabla \cdot \mathbf{v})^2$ . Replacing the last term in equation 32 with expression 33 results in

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) - \frac{\partial q_{ri}}{\partial x_i} + q''' - p \left( \nabla \cdot \mathbf{v} \right) + \lambda \left( \nabla \cdot \mathbf{v} \right)^2 + \mu \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \frac{\partial v_j}{\partial x_i}$$
(34)

The last two terms in (34) are usually combined into the **dissipation function**  $\Phi$ ,

$$\Phi = \lambda \left( \nabla \cdot \mathbf{v} \right)^2 + \mu \left( \frac{\partial v_i}{\partial x_j} \frac{\partial v_j}{\partial x_i} + \frac{\partial v_j}{\partial x_i} \frac{\partial v_j}{\partial x_i} \right)$$
(35)

or, summing over the *i* and *j* indices,

$$\Phi = \lambda \left( \nabla \cdot \mathbf{v} \right)^{2} + 2\mu \left[ \left( \frac{\partial v_{1}}{\partial x_{1}} \right)^{2} + \left( \frac{\partial v_{2}}{\partial x_{2}} \right)^{2} + \left( \frac{\partial v_{3}}{\partial x_{3}} \right)^{2} \right] + \mu \left[ \left( \frac{\partial v_{1}}{\partial x_{2}} + \frac{\partial v_{2}}{\partial x_{1}} \right)^{2} + \left( \frac{\partial v_{2}}{\partial x_{3}} + \frac{\partial v_{3}}{\partial x_{2}} \right)^{2} + \left( \frac{\partial v_{3}}{\partial x_{1}} + \frac{\partial v_{1}}{\partial x_{3}} \right)^{2} \right]$$
(36)

In equation 36, the dissipation function was expanded by summing over both i and j indices in equation 35. Using the dissipation function, equation 34 is written,

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) - \frac{\partial q_{ri}}{\partial x_i} + q^{\prime\prime\prime} - p \left( \nabla \cdot \mathbf{v} \right) + \Phi$$
(37)

or

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = \nabla \cdot k \nabla T - \nabla \cdot \mathbf{q}_{\mathrm{r}} + q^{'''} - p \left(\nabla \cdot \mathbf{v}\right) + \Phi$$
(38)

Note that, without invoking Newtonian fluid behavior, the dissipation function could have been more generally stated using tensor notation as

$$\Phi = \mathbf{\sigma} : \mathbf{e} + p \nabla \mathbf{v} \tag{38b}$$

where **e** is the rate of strain tensor from Handout 6,  $\mathbf{e} = (1/2)(\nabla \mathbf{v} + \nabla \mathbf{v}^{T})$ .

Equation (38) states that the rate of change of internal energy of a fluid element moving with the flow (left hand side) equals the sum of:

1st term on right: the rate of heat flow into the element by conduction

<u>2nd term on right</u>: the rate of heat flow into the element by radiation. If there is no net absorption or emission of electromagnetic radiation within the fluid element, the term  $\nabla \cdot \mathbf{q}_r$  is zero.

<u>3rd term on right</u>: the rate at which heat is generated inside the element by an externally coupled mechanism such as a heating coil or wire, for example. There is an obvious conceptual difficulty with this term: how exactly does one fit a heating coil into an infinitesimal fluid element? Therefore, it may be tempting to drop this term from the differential balance. On the other hand, if one applies the differential energy balance to the interior of a piece of electrical wire, for example, in which local heat generation occurs due to resistive dissipation of electrical energy, then this term makes perfect sense. Therefore, we will keep it.

<u>4th term on right</u>: the rate at which pressure forces do compressive work on the fluid element (also referred to as P-V work). Recall that  $-\nabla \cdot \mathbf{v}$  is the rate of compression of the fluid element; this allows the 4th term to be identified as the rate at which compressive work is done on the fluid element by pressure forces. The compressive work is *reversible* in that it could be recovered; for instance, by re-expanding the fluid element to do work on its surroundings.

<u>5th term on right</u>: the rate at which work performed on the fluid element by viscous stresses is dissipated to internal energy by friction in the fluid. This term can be identified as such by making a connection with the 2nd Law of Thermodynamics (see below). In thermodynamic terminology, this is *irreversible* rate of work. This is the rate at which work is converted to heat. Since, according to the 2nd Law of Thermodynamics, heat cannot be fully converted back to work this process is irreversible.

From equation 36, we see that all terms in  $\Phi$  are derived from the presence of velocity gradients (i.e. relative rate of separation of different parts of the fluid) and that  $\Phi$  must always be greater than zero,  $\Phi > 0$ . (Can you explain why there is no dissipation term in the total energy balance, equation 16?).

The units of all the terms in equation 38 are energy/(volume time).

For some materials, such as ideal gases and strictly incompressible liquids and solids, the internal energy *u* is only a function of temperature so that u = u(T). In that case, the **constant volume specific heat capacity**  $\hat{c}_V$  is defined by

$$\hat{c}_{\rm V} = {\rm d}u/{\rm d}T \tag{39}$$

so that

$$\mathrm{d}u = \hat{c}_{\mathrm{V}} \,\mathrm{d}T \tag{40}$$

Using equation 40, the rate of change of the internal energy of a fluid element moving with the flow, Du/Dt, is equal to

$$Du/Dt = \hat{c}_V DT/Dt$$
 (ideal gases or incompressible liquids) (41)

where DT/Dt is the rate of temperature change of the fluid element. Using equation (41), the internal energy balance (equation 38) becomes

$$\rho \hat{c}_V \frac{\mathrm{D}T}{\mathrm{D}t} = \nabla \cdot k \nabla T - \nabla \cdot \mathbf{q}_r + q^{'''} - p \left(\nabla \cdot \mathbf{v}\right) + \Phi \quad \text{(ideal gases or incompressible liquids)}$$
(42)

or, if the substantial derivative is expanded,

$$\rho \hat{c}_V \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = \nabla \cdot k \nabla T - \nabla \cdot \mathbf{q}_r + q''' - p \left( \nabla \cdot \mathbf{v} \right) + \Phi$$
(43)  
(ideal areas or incompressible liquids)

(ideal gases or incompressible liquids)

After much manipulation, we have arrived at a useful form of the energy balance that will allow us to calculate temperature fields, a quantity of great engineering importance.

In this course we will mostly be concerned with incompressible liquids or solids, or ideal gases, so that equations 42 and 43 apply. However, we make a few brief comments about the case when these equations are not good approximations because the internal energy depends on other variables besides temperature. For instance, for single component systems (e.g. pure fluids) that are compressible, *u* becomes a function of two variables such as *T* and the density  $\rho$ . The dependence on  $\rho$  is usually expressed in terms of  $1/\rho$ , the volume of fluid per unit mass of fluid.  $1/\rho$  is customarily referred to as the "**specific volume**" V. If u = u(T, V), then  $du = (\partial u/\partial T)_V dT + (\partial u/\partial V)_T dV$ . By definition, the derivative  $(\partial u/\partial T)_V = \hat{c}_V$ ; therefore  $du = \hat{c}_V dT + (\partial u/\partial V)_T dV$ . Thus, when *u* depends on V as well as *T*, equation 42 gets a term corresponding to the  $(\partial u/\partial V)_T$  dependence,

$$\rho \left( \hat{c}_{V} \frac{\mathrm{D}T}{\mathrm{D}t} + \left( \frac{\partial u}{\partial V} \right)_{T} \frac{\mathrm{D}V}{\mathrm{D}t} \right) = \nabla \cdot k \nabla T - \nabla \cdot \mathbf{q}_{r} + q''' - p \left( \nabla \cdot \mathbf{v} \right) + \Phi$$
(44)

If needed, the term  $(\partial u / \partial V)_T D V / Dt$  can be further rearranged using thermodynamic identities.

For many common situations equations 42 and 43 simplify into more user friendly forms. For example, typically the rate of heat absorption or emission by radiation is negligible, so that  $\nabla \cdot \mathbf{q}_r \approx 0$ . Moreover, when there is no heat generation in the material by externally-coupled processes q''' = 0, and if the thermal conductivity k is assumed constant then k can be taken outside the  $\nabla$  operator. So, for example, under these circumstances equation 43 rearranges to

$$\rho \hat{c}_V \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = k \nabla \cdot \nabla T - p \left( \nabla \cdot \mathbf{v} \right) + \Phi = k \nabla^2 T - p \left( \nabla \cdot \mathbf{v} \right) + \Phi$$
(45)  
(*k* constant; *q*<sup>'''</sup> = 0; no radiative processes)

Furthermore, if the flow is incompressible so that  $\rho = \text{constant}$ , the  $\nabla \cdot \mathbf{v}$  terms in equation 43 and in the dissipation function equation 36 disappear. Thus

$$\rho \hat{c}_V \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = k \nabla^2 T + \Phi \qquad (\rho, k \text{ constant}; q''' = 0; \text{ no radiative processes}) \qquad (46)$$

where  $\Phi$  is given by equation 36 but without the  $\nabla \cdot \mathbf{v}$  term. If, in addition, we are considering the temperature distribution in a solid material or a fluid at rest, then  $\mathbf{v} = \mathbf{0}$ . When  $\mathbf{v} = 0$ ,  $\Phi$  also equals zero (see equation 36), and equation 46 becomes

$$\frac{\partial T}{\partial t} = \frac{k}{\rho \hat{c}_V} \nabla^2 T \qquad (\rho, k \text{ constant}; \mathbf{v} = \mathbf{0}; q^m = 0; \text{ no radiative processes}) \qquad (47)$$

For strictly incompressible solids and liquids the density does not depend on temperature, and the constant volume and **constant pressure** specific heat capacities are equal,  $\hat{c}_V = \hat{c}_P$  (one could prove this from thermodynamic relations and the definitions of  $\hat{c}_V$  and  $\hat{c}_P$ ). Since most *solids and liquids* typically do not expand very much with temperature this equality is often an excellent approximation, so that  $\hat{c}_P$  can be used instead of  $\hat{c}_V$  in the above equations. If  $\hat{c}_P$  is used instead of  $\hat{c}_V$  in equation 47, the combination of parameters in front of  $\nabla^2 T$  would be  $k/\rho \hat{c}_P$ . This particular combination is referred to as the **thermal diffusivity**  $\alpha$ ,

$$\alpha = k/\rho \hat{c}_{\rm P} \tag{48}$$

and 47 may be written as

<u>)</u>

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T \qquad (\rho, k \text{ constant}; \mathbf{v} = \mathbf{0}; q''' = 0; \text{ no radiative processes}; \hat{c}_{\rm V} = \hat{c}_{\rm P}) \qquad (49)$$

Other simplifications of the energy balance, in addition to the examples above, are possible. Of course, in any problem the simplifications must reflect the physical nature and statement of the problem.

**Remarks on the 2nd Law of Thermodynamics and the conservation laws.** From thermodynamics, the entropy change of a system, dS, that results from a process involving the system must be greater than or equal to dQ/T, where dQ is the heat transferred from surroundings to the system and *T* is the absolute temperature of the system. Therefore,

$$\mathrm{d}S \ge \mathrm{d}Q/T \tag{50}$$

Applying equation 50 to a fixed, open control volume through which material can flow (i.e. the control volume is the "system") leads to

$$\frac{d}{dt} \int_{V} s\rho dV \ge -\int_{A} s\rho(\mathbf{n} \cdot \mathbf{v}) dA - \int_{A} \mathbf{n} \cdot \frac{\mathbf{q}}{T} dA$$
(51)

where *s* is entropy per mass of material (specific entropy), *V* is the control volume, *A* is the surface enclosing the control volume, **n** is the outward unit normal to *A*, **v** is the flow velocity, and **q** is the heat flux. Equation 51 is a macroscopic balance on entropy which states that the rate of accumulation of entropy inside the control volume (left hand side) must be greater than or equal to the convection of entropy into the control volume by fluid flow (1st term on right) plus the rate of heat flux into the control volume divided by *T* (2nd term on right). The equality in equation 51 would apply if all transport processes occurring within the system were reversible. All real processes are irreversible to some extent, so that entropy is generated as a consequence. If we introduce the rate of entropy generation per mass s''', to account for this generation of entropy, we can convert expression 51 to an equality,

$$\frac{d}{dt} \int_{V} s\rho dV = -\int_{A} s\rho(\mathbf{n} \cdot \mathbf{v}) dA - \int_{A} \mathbf{n} \cdot \frac{\mathbf{q}}{T} dA + \int_{V} s''' \rho dV$$
(52)

Applying the divergence theorem and collecting all terms under a single integral over V,

$$\int_{V} \left( \frac{\partial(s\rho)}{\partial t} - s'''\rho + \nabla \cdot s\rho \mathbf{v} + \nabla \cdot \frac{\mathbf{q}}{T} \right) dV = 0$$
(53)

from which the differential balance on entropy is obtained

$$\frac{\partial(s\rho)}{\partial t} - s'''\rho + \nabla \cdot s\rho \mathbf{v} + \nabla \cdot \frac{\mathbf{q}}{T} = 0$$
(54)

Alternately, using the product rule of differentiation, we can write

$$s\frac{\partial\rho}{\partial t} + \rho\frac{\partial s}{\partial t} + s(\nabla \cdot \rho \mathbf{v}) + \rho \mathbf{v} \cdot \nabla s - s'''\rho + \nabla \cdot \frac{\mathbf{q}}{T} = 0$$
(55)

The sum of the first and third terms, according to the equation of continuity (equation 1), is zero. Therefore, we are left with

$$\rho \frac{\partial s}{\partial t} + \rho \mathbf{v} \cdot \nabla s - s''' \rho + \nabla \cdot \frac{\mathbf{q}}{T} = 0$$
(56)

$$\rho \frac{\mathrm{D}s}{\mathrm{D}t} = s''' \rho - \nabla \cdot \left(\frac{\mathbf{q}}{T}\right) \tag{57}$$

Note that equation 57 is written for a *closed* system (i.e. a fluid element moving with the flow into which there is no convection). From thermodynamics, we recall that for a closed system

$$du = Tds - pdV$$

where V is the specific volume. If the above expression is applied to a fluid element moving with the flow, it reads

$$\rho \frac{\mathrm{D}u}{\mathrm{D}t} = \rho T \frac{\mathrm{D}s}{\mathrm{D}t} - p\rho \frac{\mathrm{D}V}{\mathrm{D}t} = \rho T \frac{\mathrm{D}s}{\mathrm{D}t} - p\rho \frac{\mathrm{D}(1/\rho)}{\mathrm{D}t} = \rho T \frac{\mathrm{D}s}{\mathrm{D}t} + \frac{p}{\rho} \frac{\mathrm{D}\rho}{\mathrm{D}t} = \rho T \frac{\mathrm{D}s}{\mathrm{D}t} - p(\nabla \cdot \mathbf{v})$$
(58)

where equation 1 was used after the last "=" sign in equation 58. Therefore,

$$\rho T \frac{\mathrm{D}s}{\mathrm{D}t} = \rho \frac{\mathrm{D}u}{\mathrm{D}t} + p(\nabla \cdot \mathbf{v})$$
(59)

Substituting equation 57 for the left hand side in equation 59, and equation 38 for the first term on the right,

$$Ts'''\rho - T\nabla \cdot \left(\frac{\mathbf{q}}{T}\right) = \nabla \cdot k\nabla T - \nabla \cdot \mathbf{q}_r + q''' + \Phi$$
(60)

Splitting the heat transfer **q** into conductive (according to Fourier's Law) and radiative parts,  $\mathbf{q} = \mathbf{q}_{\rm C} + \mathbf{q}_{\rm r} = -k\nabla T + \mathbf{q}_{\rm r}$  rearranges equation 60 into

$$s'''\rho + \nabla \cdot \left(\frac{k\nabla T}{T}\right) - \nabla \cdot \left(\frac{\mathbf{q}_r}{T}\right) = \frac{1}{T} \nabla \cdot k \nabla T - \frac{1}{T} \nabla \cdot \mathbf{q}_r + \frac{q'''}{T} + \frac{\Phi}{T}$$
(61)

Now,

$$\nabla \cdot \left(\frac{k\nabla T}{T}\right) = \frac{1}{T} \nabla \cdot k\nabla T + k\nabla T \cdot \nabla \frac{1}{T} = \frac{1}{T} \nabla \cdot k\nabla T - \frac{k\nabla T}{T^2} \cdot \nabla T = \frac{1}{T} \nabla \cdot k\nabla T - \frac{k(\nabla T)^2}{T^2}$$
(62)

and

$$-\nabla \cdot \left(\frac{\mathbf{q}_{r}}{T}\right) = -\frac{1}{T} \nabla \cdot \mathbf{q}_{r} - \mathbf{q}_{r} \cdot \nabla \left(\frac{1}{T}\right) = -\frac{1}{T} \nabla \cdot \mathbf{q}_{r} + \frac{\mathbf{q}_{r}}{T^{2}} \cdot \nabla T$$
(63)

Inserting equations 62 and 63 into equation 61 and simplifying,

$$s'''\rho = \frac{k(\nabla T)^2}{T^2} - \frac{\mathbf{q}_r}{T^2} \cdot \nabla T + \frac{q'''}{T} + \frac{\Phi}{T}$$
(64)

Equation 64 shows that the rate of entropy production per unit volume,  $s'''\rho$ , results from irreversibilities due to the presence of temperature gradients (1st term on right), generation of heat by externally coupled processes (3rd term on right), presence of frictional dissipation of mechanical energy to heat due to "rubbing" because of velocity gradients (4th term on right), and coupling between the temperature and electromagnetic radiation fields (2nd term on right). The most important conclusion from equation 64 is that presence of velocity gradients, as captured by the dissipation function  $\Phi$ , and of temperature gradients associated with heat conduction, always lead to positive generation of entropy and hence represent irreversibilities associated with the transport of momentum and energy.

**Remarks on ''Conduction of momentum.''** In equation 46, assuming constant value of the thermal conductivity *k*, heat conduction was represented by the term  $k\nabla^2 T$ . In the Navier-Stokes equations, equation 15, under assumption of constant viscosity  $\mu$  there was a term  $\mu\nabla^2 \mathbf{v}$ . Let's compare the meaning of these two terms.

The heat conduction term represents transfer of heat by molecular level processes. Imagine a control volume - how is heat conducted from one side of the control volume surface to the other by "molecular level processes"? Molecular level processes include molecular collisions that transfer energy from more agitated (hotter) to less agitated (cooler) molecules. As such collisions will occur across the control volume surface even if there is no bulk convection, this transfer is one example of heat flow by conduction. It is also possible that hotter molecules from one side of a control volume enter while colder molecules leave from the other side. If this "molecular exchange" is such that the local average velocity (i.e. the average velocity of all the molecules crossing the control volume surface at the point of interest) is zero normal to the surface, then this transfer is also not convective since there is no bulk flow across the surface. Then the transfer is viewed as conductive. The sum total of all conductive processes, whatever their physical origin, is represented by the conductive heat flux  $\mathbf{q}_{\rm C}$  that follows Fourier's Law,  $\mathbf{q}_{\rm C} = -k\nabla T$ . From this expression, it is seen that temperature gradients are the "driving force" for heat conduction. If there are no temperature gradients, there is no heat conduction.

How is momentum transferred by molecular level processes? Faster molecules on one side of a control volume surface can collide with slower molecules on the other side, thus transferring momentum across the surface. This momentum transfer could be considered "conductive" since no molecules crossed across the control volume surface. It is also possible that faster molecules cross the control volume surface in one direction while slower molecules cross in the other direction such that the net average velocity is zero normal to the surface. Again, since there is no bulk convection, such

transfer of momentum could be termed to be "conductive." Because the term  $\mu \nabla^2 \mathbf{v}$  in equation 15 represents such molecular level processes, it is at times referred to as "conduction of momentum." Note that if there are no velocity gradients, there is no conduction of momentum.

# **Common Boundary Conditions**

Integration of differential equations leads to the appearance of integration constants. The differential equations of transport phenomena that we have been studying are no exception to this rule. The integration constants are typically evaluated using "**boundary**" or "**initial**" conditions. Boundary conditions make a physical statement that is believed to be true and that we want to enforce at some location within the system (often, the location is the system boundary). Initial conditions represent a physical statement that we want to enforce at some point in time (often, the time is the starting or initial time of a process). Some of the more common boundary and initial conditions encountered when solving the differential equations of transport phenomena are discussed below.

1). Initial conditions. Examples:

$$\mathbf{v}(t=0) = \mathbf{v}_0 \tag{65}$$

$$T(t=0) = T_0$$
(66)

where  $\mathbf{v}_0$  and  $T_0$  are known constants or functions of variables other than *t*. For example, we could have  $T_0 = f(\mathbf{r})$  if  $T_0$  depends on position.

**2). Impenetrable boundary**. This boundary condition expresses the fact that material is not allowed to move across an impenetrable boundary. Thus, at the boundary, we must have

$$\mathbf{v} \cdot \mathbf{n} = \mathbf{v}_{\perp} = \mathbf{0} \tag{67}$$

where **v** is the material velocity, **n** is a unit normal to the boundary, and  $v_{\perp}$  is the component of **v** perpendicular to the boundary.

**3). The ''no-slip'' boundary condition.** This boundary condition assumes that material on both sides of a boundary between two physical phases moves with the same velocity. For example, fluid right next to a stationary solid wall is assumed to be stationary, while fluid right next to a moving solid wall is assumed to move with the same velocity as the wall. Similarly, at the boundary between two immiscible fluids I and II, the velocity of fluid I immediately on one side of the boundary is assumed to equal that of fluid II immediately on the other side. Mathematically, the no-slip condition can be represented as

$$\mathbf{v}_{\mathrm{I}} = \mathbf{v}_{\mathrm{II}} \tag{68}$$

where  $v_I$  and  $v_{II}$  are the velocities of material at the boundary between phases I and II, respectively.

**4). Continuity of stress across a boundary (at** *planar* **boundaries with uniform conditions)**. In this boundary condition, the stress (normal and shear) exerted by material on one side of a boundary is assumed to be equal and opposite to that exerted by the material on the other side. This statement is not always true, and in fact if the boundary is curved (recall: what happens if a surface is curved?), or if

there are variations in the conditions at the boundary (e.g. due to composition or temperature changes) then surface tension effects arise which must also be accounted for. We will assume that the boundaries are planar, and that the conditions at the boundary are the same everywhere. In such a simplified scenario, the mathematical statement of the existence of equal and opposite stresses on the two sides of a boundary can be written

$$\mathbf{n} \cdot \boldsymbol{\sigma} = -\mathbf{n}_{+} \cdot \boldsymbol{\sigma}_{+} \tag{69}$$

where the subscript "-" signifies quantities on the "minus" side of (i.e. below) the boundary while "+" signifies quantities on the "plus" side of (i.e. above) the boundary.  $\mathbf{n}_{-}$  is a unit normal to the boundary pointing in the negative direction, while  $\mathbf{n}_{+}$  is a unit normal that points in the positive direction. Since  $\mathbf{n}_{-} = -\mathbf{n}_{+}$ , the above equation reduces to the simple statement

 $\boldsymbol{\sigma}_{-} = \boldsymbol{\sigma}_{+} \tag{70}$ 

Equation 70 states that the stress tensor on one side of the boundary must equal that on the other side. This means that both the normal and shear stresses are continuous (i.e. do not change) across the boundary. For the particular case when the material on one side of the boundary is a gas, because of the low viscosity of gases it is often assumed that the viscous stresses at the boundary are vanishingly small. In that case the viscous shear stresses, and viscous normal stresses (but not pressure), at the boundary are often approximated to equal zero.

**5). Continuity of stress across a boundary (general case)**. It is important to realize that all the above boundary conditions have inherent assumptions. For example, the continuity of the stress tensor can be violated by surface tension effects. The full condition on the stress tensor that also allows for surface curvature and surface tension gradients is

$$\mathbf{n}_{-} \cdot \boldsymbol{\sigma}_{-} + \mathbf{n}_{+} \cdot \boldsymbol{\sigma}_{+} + \nabla_{s} \boldsymbol{\gamma} + 2\boldsymbol{\varsigma} \boldsymbol{\gamma} \mathbf{n} = \mathbf{0}$$
(70a)

where the surface gradient operator is given by (note that this operator takes the gradient of a function within a surface)

$$\nabla_{s} = \nabla - \mathbf{n}_{+} (\mathbf{n}_{+} \cdot \nabla) \tag{70b}$$

and the surface mean curvature is calculated from

$$\boldsymbol{\varsigma} = mean\ curvature = -\frac{1}{2}\nabla_{\mathbf{s}} \cdot \mathbf{n}_{+} \tag{70c}$$

For a surface specified by z = f(x,y) in the CCS, these expressions become

$$\nabla_{\mathbf{s}} = \frac{1}{H^2} \left\{ \left[ 1 + \left( \frac{\partial f}{\partial x_2} \right)^2 \right] \mathbf{\delta}_1 - \frac{\partial f}{\partial x_1} \frac{\partial f}{\partial x_2} \mathbf{\delta}_2 + \frac{\partial f}{\partial x_1} \mathbf{\delta}_3 \right\} \frac{\partial}{\partial x_1} + \frac{1}{H^2} \left\{ -\frac{\partial f}{\partial x_1} \frac{\partial f}{\partial x_2} \mathbf{\delta}_1 + \left[ 1 + \left( \frac{\partial f}{\partial x_1} \right)^2 \right] \mathbf{\delta}_2 + \frac{\partial f}{\partial x_2} \mathbf{\delta}_3 \right\} \frac{\partial}{\partial x_2} \frac{\partial}{\partial x_2} \mathbf{\delta}_3 + \frac{\partial}{\partial x_2} \mathbf{\delta}_4 \mathbf{\delta}_3 \right\} \frac{\partial}{\partial x_2} \mathbf{\delta}_4 + \frac{\partial}{\partial x_2} \mathbf{\delta}_4 \mathbf{\delta}_4$$

$$H = \left[ \left( \frac{\partial f}{\partial x_1} \right)^2 + \left( \frac{\partial f}{\partial x_2} \right)^2 + 1 \right]^{1/2}$$
(70e)

$$\varsigma = \frac{1}{2H^3} \left\{ \left[ 1 + \left(\frac{\partial f}{\partial x_2}\right)^2 \right] \frac{\partial^2 f}{\partial x_1^2} - 2\frac{\partial f}{\partial x_1} \frac{\partial f}{\partial x_2} \frac{\partial^2 f}{\partial x_1 \partial x_2} + \left[ 1 + \left(\frac{\partial f}{\partial x_1}\right)^2 \right] \frac{\partial^2 f}{\partial x_2^2} \right\}$$
(70f)

**6). Temperature Boundary Conditions**. A very common boundary condition is one in which temperature is specified at a point in space. For example,

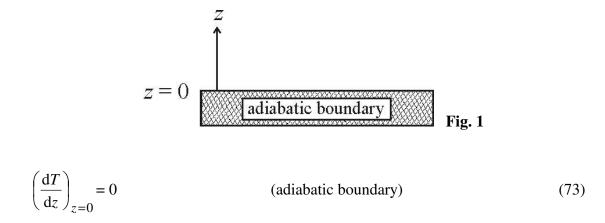
$$T\left(x=0\right) = T_{\rm o} \tag{71}$$

where the value of  $T_0$  is given (noting that  $T_0$  may be a function, for example  $T_0(t)$ ).

7). Conditions on Heat Flux. One example of a boundary condition on heat flux deals with heat conduction at an **adiabatic** boundary or wall. By definition, an adiabatic wall does not transmit heat. From Fourier's Law, the conductive heat flux  $q_{C\perp}$  normal to the boundary is given by

$$q_{\rm C\perp} = -k\nabla T_{\perp} = -k\frac{\mathrm{d}T}{\mathrm{d}z} \tag{72}$$

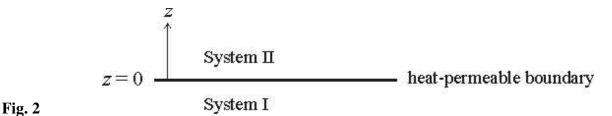
where z was taken to be the coordinate perpendicular to the boundary (Fig. 1) and the subscript " $_{\perp}$ " indicates the component of the conductive heat flux that is normal to the boundary. It will be assumed that the boundary is located at z = 0. Since the boundary is adiabatic, there can be no conductive heat flux perpendicular to it; therefore,  $q_{C\perp}$  must equal zero at z = 0. This condition implies that



The subscript z = 0 on the temperature derivative indicates that the derivative is to be evaluated right at the boundary; i.e. at z = 0.

Now imagine that we have a **heat-permeable** (diathermal) boundary between systems I and II (Fig. 2), and that steady state conditions apply. Under steady state, there can be no accumulation of heat at the boundary. If heat conduction is the only means by which heat arrives and leaves the boundary,

then the rate at which heat is conducted to the boundary from system I must equal the rate at which it is conducted away from the boundary into system II,



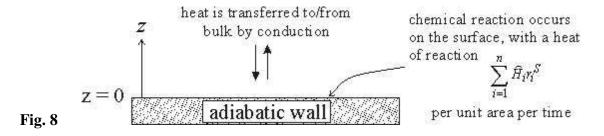
$$k_{\rm I} \left(\frac{\mathrm{d}T}{\mathrm{d}z}\right)_{\mathrm{I},z=0} = k_{\rm II} \left(\frac{\mathrm{d}T}{\mathrm{d}z}\right)_{\mathrm{II},z=0} \tag{60}$$

 $k_{\rm I}$  and  $k_{\rm II}$  are heat conductivities in systems I and II, respectively, and  $\left(\frac{\mathrm{d}T}{\mathrm{d}z}\right)_{\mathrm{I},z=0}$  and  $\left(\frac{\mathrm{d}T}{\mathrm{d}z}\right)_{\mathrm{II},z=0}$  are the temperature gradients in the two systems, measured at the boundary.

A third example we consider is that of a heterogeneous reaction occurring at a boundary between a system and an adiabatic wall (Fig. 3). Under steady state conditions there can be no accumulation of heat at the boundary; therefore, the rate at which heat of reaction is generated at the boundary must equal the rate at which it leaves. Since the wall is adiabatic, no heat can flow into the wall; thus, heat can only flow into the bulk system. If conduction is the only mechanism of heat transfer away from the surface, then,

$$\sum_{i=1}^{n} \widehat{H}_{i} r_{i}^{S} = k \left(\frac{\mathrm{d}T}{\mathrm{d}z}\right)_{z=0}$$
(74)

 $r_i^{\rm S}$  is the rate at which mass of species *i* is produced by chemical reactions at the boundary (in units of mass / (area time)), *n* is the number of species participating in the reactions, and  $\hat{H}_i$  is the specific enthalpy (units: energy / mass) of species *i*. The left hand side of equation 74 is the heat generated per area per time by chemical reactions, and the right hand side is the rate at which heat flows away from the surface by conduction. Both terms have units of energy / (area time).



The above examples have involved *conduction* of heat to or from a boundary as the dominant mechanism of heat transfer. Since conduction was involved, Fourier's Law was used to calculate the heat flux. However, in many cases convection may aid in removal of heat from a boundary. In such cases, it is more customary to model the heat transport using so-called **heat transfer coefficients** h,

$$q = h \left( T_{\rm S} - T_{\infty} \right) \tag{75}$$

with  $T_S$  the temperature at the boundary and  $T_{\infty}$  the temperature in the bulk of the phase to which the heat is being transferred. In the case of radiative heat transfer, expressions introduced in the prior handout could be used to also calculate radiative heat flux at a boundary.