

# Lecture 3

## Fluid Dynamics and Balance Equations for Reacting Flows

Basics: equations of continuum mechanics

- balance equations for mass and momentum
- balance equations for the energy and the chemical species

Associated with the release of thermal energy and the increase in temperature is a local decrease in density which in turn affects the momentum balance.

Therefore, **all these equations are closely coupled** to each other.

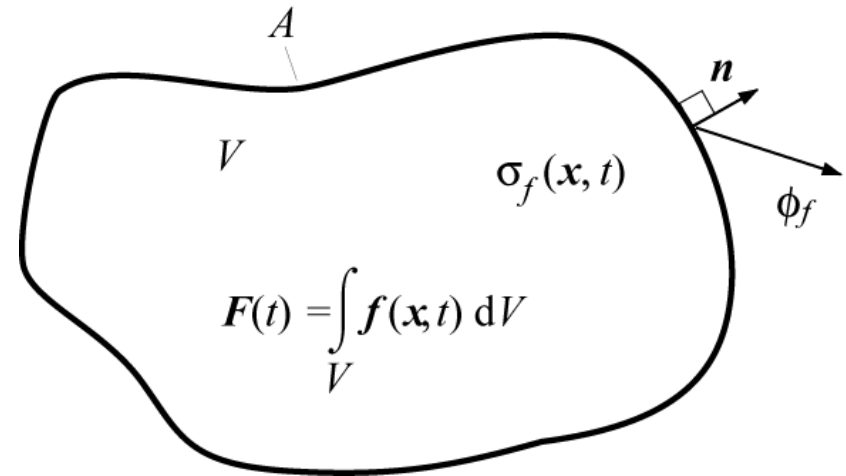
Nevertheless, in deriving these equations we will try to point out

**how they can be simplified and partially uncoupled**

under certain assumptions.

## Balance Equations

A time-independent control volume  $V$   
for a balance quality  $F(t)$



The scalar product between the **surface flux**  $\phi_f$  and the normal vector  $\mathbf{n}$  determines the outflow through the surface  $A$ , a **source**  $s_f$  the rate of production of  $F(t)$

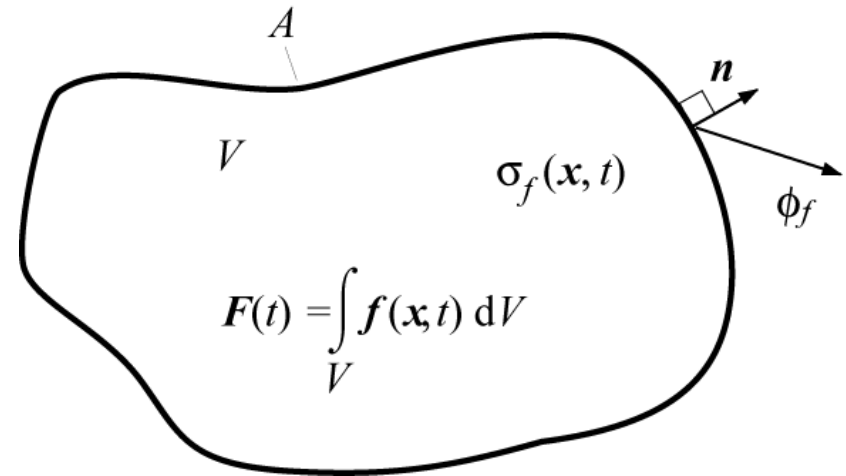
Let us consider a general quality per unit volume  $f(\mathbf{x}, t)$ .

Its integral over the finite volume  $V$ , with the time-independent boundary  $A$  is given by

$$F(t) = \int_V f(\mathbf{x}, t) dV$$

The temporal change of  $F$

$$\frac{\partial F}{\partial t} = \int_V \frac{\partial f}{\partial t} dV$$



is then due to the following three effects:

1. by the flux  $\phi_f$  across the boundary  $A$ . This flux may be due to convection or molecular transport.

By integration over the boundary  $A$  we obtain the net contribution

$$- \int_A \phi_f \cdot n dA,$$

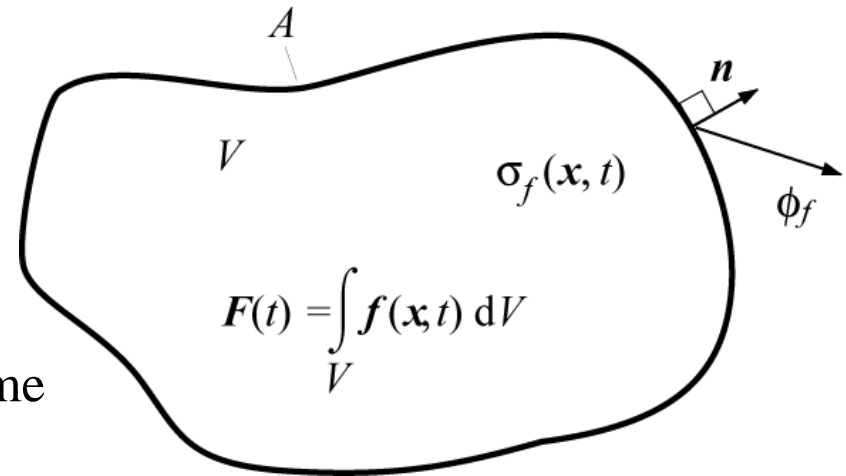
which is negative, if the normal vector is assumed to direct outwards.

2. by a local source  $\sigma_f$  within the volume.

This is an essential production of partial mass by chemical reactions.

Integrating the source term over the volume leads to

$$\int_V \sigma_f dV$$



3. by an external induced source  $s$ .

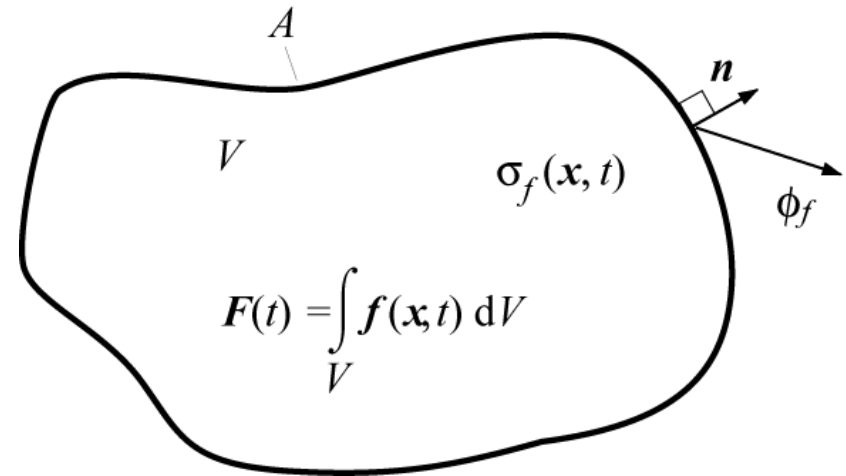
Examples are the gravitational force or thermal radiation.

Integration of  $s_f$  over the volume yields

$$\int_V s_f dV$$

We therefore have the balance equation

$$\int_V \frac{\partial f}{\partial t} dV = - \int_A \phi_f \cdot n dA + \int_V (\sigma_f + s_f) dV$$



Changing the integral over the boundary  $A$  into a volume integral using Gauss' theorem

$$\int_A \phi_f \cdot n dA = \int_V \mathbf{div} \phi_f dV$$

and realizing that the balance must be independent of the volume, we obtain the general balance equation in differential form

$$\frac{\partial f}{\partial t} = -\mathbf{div} \phi_f + \sigma_f + s_f$$

## Mass Balance

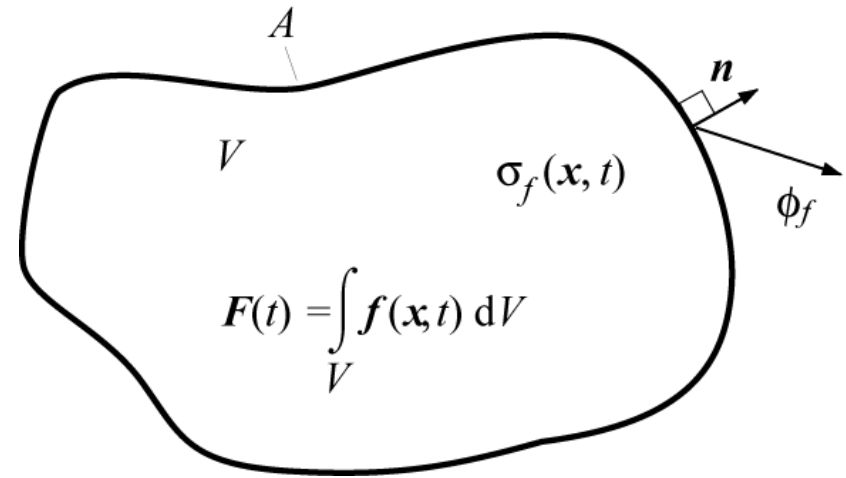
Set the partial mass per unit volume  $\rho_i = \rho Y_i = f$ .

The partial mass flux across the boundary is  $\rho_i v_i = \phi_f$ , where  $v_i$  is called the diffusion velocity.

Summation over all components yields the mass flow  $\rho v = \sum_{i=1}^k \rho_i v_i$ , where  $v$  is the mass average velocity.

The difference between  $v_i$  defines the diffusion flux  $v_i - v = \frac{j_i}{\rho_i}$ , where the sum satisfies

$$\sum_{i=1}^k j_i = 0.$$



Setting the chemical source term

$$\sigma_f = \dot{m}_i = W_i \sum_{l=1}^r \nu_{il} \omega_l$$

one obtains the **equation for the partial density**

$$\frac{\partial \rho_i}{\partial t} = -\mathbf{div}(\rho_i \mathbf{v}_i) + \dot{m}_i, \quad i = 1, 2, \dots, k.$$

The summation over  $i$  leads to the **continuity equation**

$$\frac{\partial \rho}{\partial t} = -\mathbf{div}(\rho \mathbf{v}).$$



Introducing the total derivative of a quantity  $\mathcal{A}$

$$\frac{D\mathcal{A}}{Dt} = \frac{\partial\mathcal{A}}{\partial t} + \mathbf{v} \cdot \mathbf{grad} \mathcal{A}$$

a combination with the continuity equation yields

$$\rho \frac{D\mathcal{A}}{Dt} = \frac{\partial(\rho\mathcal{A})}{\partial t} + \mathbf{div}(\rho\mathbf{v}\mathcal{A}).$$

Then  $\frac{\partial\rho_i}{\partial t} = -\mathbf{div}(\rho_i\mathbf{v}_i) + \dot{m}_i$ ,  $i = 1, 2, \dots, k$ . using  $\mathbf{v}_i - \mathbf{v} = \frac{\mathbf{j}_i}{\rho_i}$

may also be written

$$\rho \frac{DY_i}{Dt} = -\mathbf{div} \mathbf{j}_i + \dot{m}_i, \quad i = 1, 2, \dots, k.$$

## Momentum Balance

Set the momentum per unit volume  $\rho \boldsymbol{v} = \boldsymbol{f}$ .

The momentum flux is the sum of the convective momentum in flow  $\rho \boldsymbol{v} \boldsymbol{v}$  and the stress tensor

$$\boldsymbol{P} = p\boldsymbol{I} + \boldsymbol{\tau}$$

where  $\boldsymbol{I}$  is the unit tensor and  $\boldsymbol{\tau}$  is the viscous stress tensor.

Therefore  $\rho \boldsymbol{v} \boldsymbol{v} + \boldsymbol{P} = \boldsymbol{\phi}_f$ .

There is no local source of momentum, but the gravitational force from outside

$$\boldsymbol{s}_f = \rho \boldsymbol{g}$$

where  $\boldsymbol{g}$  denotes the constant of gravity.

The momentum equation then reads

$$\frac{\partial \rho \mathbf{v}}{\partial t} = -\mathbf{div} (\rho \mathbf{v} \mathbf{v} + \mathbf{P}) + \rho \mathbf{g}$$

or with  $\rho \frac{D\mathcal{A}}{Dt} = \frac{\partial(\rho \mathcal{A})}{\partial t} + \mathbf{div} (\rho \mathbf{v} \mathcal{A})$  for  $\mathcal{A} \equiv \mathbf{v}$

we obtain

$$\rho \frac{D\mathbf{v}}{Dt} = -\mathbf{grad} p - \mathbf{div} \boldsymbol{\tau} + \rho \mathbf{g}.$$

## Kinetic Energy Balance

The scalar product of the momentum equation

$$\frac{\partial \rho v}{\partial t} = -\mathbf{div}(\rho v v + P) + \rho g$$

with  $v$  provides the balance for the kinetic energy

$$\frac{1}{2} \frac{\partial}{\partial t}(\rho v^2) = -\mathbf{div}(P \cdot v + \frac{1}{2} v \rho v^2) + P : \mathbf{grad} v + \rho g \cdot v,$$

where  $v^2 = v \cdot v$ .

## Potential Energy Balance

The gravitational force may be written as the derivative of the time-independent potential

$$\mathbf{g} = -\mathbf{grad} \psi, \quad \frac{\partial \psi}{\partial t} = 0.$$

Then with the continuity equation

$$\frac{\partial \rho}{\partial t} = -\mathbf{div}(\rho \mathbf{v})$$

the balance for the potential energy is

$$\frac{\partial(\rho\psi)}{\partial t} = -\mathbf{div}(\rho \mathbf{v} \psi) - \rho \mathbf{g} \cdot \mathbf{v}.$$

## Total and Internal Energy and Enthalpy Balance

The first law of thermodynamics states that the total energy must be conserved, such that the local source  $\sigma_f = 0$ .

We set  $\rho e = f$ , where the total energy per unit mass is

$$e = u + \frac{1}{2}v^2 + \psi.$$

This defines the internal energy introduced in

$$du + pdv = dh - vdp = \delta q + \delta w_R$$

The total energy flux  $\phi_f \equiv \mathbf{j}_e$  is

$$\mathbf{j}_e = \rho e \mathbf{v} + \mathbf{P} \cdot \mathbf{v} + \mathbf{j}_q$$

which defines the total heat flux  $\mathbf{j}_q$ .

The externally induced source due to radiation is  $\dot{q}_R = s_f$

Then the total energy balance  $\frac{\partial(\rho e)}{\partial t} = -\mathbf{div} \mathbf{j}_e + \dot{q}_R$

may be used to derive an equation for the internal energy

$$\frac{\partial(\rho u)}{\partial t} = -\mathbf{div} (\rho \mathbf{v} u + \mathbf{j}_q) - \mathbf{P} : \mathbf{grad} \mathbf{v} + \dot{q}_R.$$

Using  $\rho \frac{D\mathcal{A}}{Dt} = \frac{\partial(\rho\mathcal{A})}{\partial t} + \mathbf{div}(\rho\mathbf{v}\mathcal{A})$

this may be written with the total derivative

$$\rho \frac{Du}{Dt} = -\mathbf{div} \mathbf{j}_q - p \mathbf{div} \mathbf{v} + \boldsymbol{\tau} : \mathbf{grad} \mathbf{v} + \dot{q}_R$$

With the continuity equation  $\frac{\partial \rho}{\partial t} = -\mathbf{div}(\rho\mathbf{v})$ .

we may substitute  $\mathbf{div} \mathbf{v} = \rho \frac{D}{Dt} \left( \frac{1}{\rho} \right)$

to find

$$\underbrace{\frac{Du}{Dt}}_{\propto du} + \underbrace{p \frac{D}{Dt} \left( \frac{1}{\rho} \right)}_{\propto p dv} = \underbrace{\frac{1}{\rho} \left[ -\mathbf{div} \mathbf{j}_q + \dot{q}_R \right]}_{\propto \delta q} + \underbrace{\frac{1}{\rho} \boldsymbol{\tau} : \mathbf{grad} \mathbf{v}}_{\propto \delta w_R}$$

illustrating the equivalence with the first law introduced in a global thermodynamic balance.



With the enthalpy  $h = u + p/\rho$  the energy balance equation can be formulated for the enthalpy

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} = -\mathbf{div} \mathbf{j}_q + \boldsymbol{\tau} : \mathbf{grad} \mathbf{v} + \dot{q}_R.$$

## Transport Processes

In its most general form **Newton's law** states that the viscous stress tensor is proportional to the symmetric, trace-free part of the velocity gradient

$$\boldsymbol{\tau} = -\mu \left[ \mathbf{grad} \, \boldsymbol{v} - \frac{\mathbf{div} \, \boldsymbol{v}}{3} \boldsymbol{I} \right]^{\text{sym}}$$

Here the suffix <sup>sym</sup> denotes that only the symmetric part is taken and the second term in the brackets subtracts the trace elements from the tensor.

Newton's law thereby defines the **dynamic viscosity**.

Similarly **Fick's law** states that the diffusion flux is proportional to the concentration gradient.

Due to thermodiffusion it is also proportional to the temperature gradient.

The most general form for multicomponent diffusion is written as

$$\mathbf{j}_i = \frac{W_i}{W} \sum_{\substack{j=1 \\ j \neq i}}^k \rho D_{ij} W_j \mathbf{grad} X_j - \frac{D_i^T}{T} \mathbf{grad} T, \quad i = 1, 2, \dots, k.$$

For most combustion processes thermodiffusion can safely be neglected.

For a binary mixture Fick's law reduces to

$$\mathbf{j}_i = -\rho D_{ij} \mathbf{grad} Y_i$$

where  $D_{ij} = D_{ji}$  is the **binary diffusion coefficient**.

For multicomponent mixtures, where one component occurs in large amounts, as for the combustion in air where **nitrogen is abundant**, all other species may be treated as trace species and

$$j_i = -\rho D_i \mathbf{grad} Y_i, \quad D_i = D_{i,N_2}$$

with the binary diffusion coefficient with respect to the abundant component may be used as an approximation

A generalization for an **effective diffusion coefficient**  $D_i$  to be used for the minor species is

$$D_i = \frac{\sum_{\substack{i=1 \\ i \neq j}}^k X_i}{\sum_{\substack{j=1 \\ j \neq i}}^k X_j / D_{ij}}$$

Note that the use of

$$\mathbf{j}_i = -\rho D_i \mathbf{grad} Y_i, \quad D_i = D_{i,N_2}$$

does not satisfy the condition  $\sum_{i=1}^k \mathbf{j}_i = \mathbf{0}$ .

Finally, **Fourier's law** of thermal conductivity states that the heat flux should be proportional to the negative temperature gradient.

The heat flux  $\mathbf{j}_q$  includes the effect of partial enthalpy transport by diffusion and is written

$$\mathbf{j}_q = -\lambda \mathbf{grad} T + \sum_{i=1}^k h_i \mathbf{j}_i$$

which defines the **thermal conductivity**  $\lambda$ .

In Fourier's law

$$\mathbf{j}_q = -\lambda \mathbf{grad} T + \sum_{i=1}^k h_i \mathbf{j}_i$$

the Dufour heat flux has been neglected.

Transport coefficients for single components can be calculated on the basis of the theory of rarefied gases.

## Different forms of the energy equation

We start from the enthalpy equation

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} = -\mathbf{div} \mathbf{j}_q + \boldsymbol{\tau} : \mathbf{grad} \mathbf{v} + \dot{q}_R.$$

and neglect in the following the viscous dissipation term and the radiative heat transfer term.

Then, differentiating  $h = \sum_{i=1}^k Y_i h_i$  yields

$$dh = c_p dT + \sum_{i=1}^k h_i dY_i,$$

where  $c_p$  is the heat capacity at constant pressure of the mixture.

We can write the heat flux as

$$\mathbf{j}_q = -\frac{\lambda}{c_p} \mathbf{grad} h + \sum_{i=1}^k h_i \left( \mathbf{j}_i + \frac{\lambda}{c_p} \mathbf{grad} Y_i \right).$$

If the diffusion flux can be approximated by

$$\mathbf{j}_i = -\rho D_{ij} \mathbf{grad} Y_i = -\rho D_i \mathbf{grad} Y_i$$

with an effective diffusion coefficient  $D_i$ , we introduce the Lewis number

$$\text{Le}_i = \frac{\lambda}{\rho c_p D_i}$$

and write the last term as

$$\sum_{i=1}^k h_i \left( \mathbf{j}_i + \frac{\lambda}{c_p} \mathbf{grad} Y_i \right) = \sum_{i=1}^k h_i \left( 1 - \frac{1}{\text{Le}_i} \right) \frac{\lambda}{c_p} \mathbf{grad} Y_i$$

This term vanishes if the Lewis numbers of all species can be assumed equal to unity.



This is an interesting approximation because it leads to the following form of the enthalpy

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} h \right).$$

If the  $p = \text{const}$  as it is approximately the case in all applications except in reciprocating engines, the enthalpy equation would be very much simplified.

The assumption  $Le=1$  for all species is not justified in many combustion applications.

In fact, deviations from that assumption lead to a number of interesting phenomena that have been studied recently in the context of flame stability and the response of flames to external disturbances.

We will address these questions in some of the lectures below.

Another important form of the energy equation is that in terms of the temperature.

With

$$dh = c_p dT + \sum_{i=1}^k h_i dY_i,$$

and

$$\rho \frac{DY_i}{Dt} = -\mathbf{div} \mathbf{j}_i + \dot{m}_i, \quad i = 1, 2, \dots, k.$$

the total derivative of the enthalpy can be written as

$$\rho \frac{Dh}{Dt} = \rho c_p \frac{DT}{Dt} + \sum_{i=1}^k (-\mathbf{div} \mathbf{j}_i + \dot{m}_i) h_i.$$

Then with

$$\mathbf{j}_q = -\lambda \mathbf{grad} T + \sum_{i=1}^k h_i \mathbf{j}_i$$

the enthalpy equation

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} = -\mathbf{div} \mathbf{j}_q + \boldsymbol{\tau} : \mathbf{grad} \mathbf{v} + \dot{q}_R.$$

without the second last term yields the temperature equation

$$\rho c_p \frac{DT}{Dt} + \mathbf{div} (\lambda \mathbf{grad} T) - \sum_{i=1}^k c_{pi} \mathbf{j}_i \cdot \mathbf{grad} T - \sum_{i=1}^k \dot{m}_i h_i + \dot{q}_R$$

Here the last term describes the temperature change due to chemical reactions.

It may be written as

$$-\sum_{i=1}^k \dot{m}_i h_i = -\sum_{l=1}^r \sum_{i=1}^k \nu_{il} W_i h_i \omega_l = \sum_{l=1}^r Q_l \omega_l$$

where the definition

$$a_l = -\sum_{i=1}^k \nu_{il} W_i h_i = -\sum_{i=1}^k \nu_{il} H_i$$

has been used for each reaction.

The second term on the right hand side may be neglected, if one assumes that all specific heats  $c_{pi}$  are equal.

This assumption is very often justified since this term does not contribute as much to the change of temperature as the other terms in the equation, in particular the chemical source term.

If one also assumes that spatial gradients of  $c_p$  may be neglected for the same reason, the temperature equation takes the form

$$\rho \frac{DT}{Dt} = \frac{1}{c_p} \frac{Dp}{Dt} + \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} T \right) + \sum_{l=1}^r \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p}.$$

For a constant pressure it is very similar to the equation for the mass fraction  $Y_i$  with an equal diffusion coefficient  $D = \lambda / \rho / c_p$  for all reactive species and a spatially constant Lewis number may be written as

$$\rho \frac{DY_i}{Dt} = \frac{1}{Le_i} \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Y_i \right) + W_i \sum_{l=1}^r \nu_{il} \omega_l.$$

## Lewis numbers of some reacting species occurring in methane-air flames

CH <sub>4</sub>	O <sub>2</sub>	H <sub>2</sub> O	CO <sub>2</sub>	H	O	OH	HO <sub>2</sub>
0.97	1.11	0.83	1.39	0.18	0.70	0.73	1.10

H <sub>2</sub>	CO	H <sub>2</sub> O <sub>2</sub>	HCO	CH <sub>2</sub> O	CH <sub>3</sub>	CH <sub>3</sub> O
0.3	1.10	1.12	1.27	1.28	1.00	1.30

For  $Le_i=1$  the species transport equation and the temperature equation are easily combined to obtain the enthalpy equation.

Since the use of 
$$\rho \frac{DT}{Dt} = \frac{1}{c_p} \frac{Dp}{Dt} + \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} T \right) + \sum_{l=1}^r \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p}$$

and 
$$\rho \frac{DY_i}{Dt} = \frac{1}{Le_i} \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Y_i \right) + W_i \sum_{l=1}^r \nu_{il} \omega_l$$

does not require the  $Le=1$  assumption, this formulation is often used when non-unity Lewis number effects are to be analyzed.

For flame calculations a sufficiently accurate approximation for the transport properties is [Smooke]

$$\frac{\lambda}{c_p} = 2.58 \cdot 10^{-4} \frac{\text{g}}{\text{cm sec}} \left( \frac{T}{298 \text{ K}} \right)^{0.7},$$

a constant Prandtl number  $Pr = \frac{\mu c_p}{\lambda} = 0.75,$

and constant Lewis numbers.  $Le_i = \frac{\lambda}{\rho c_p D_i}$

A first approximation for other hydrocarbon species can be based on the assumption that the binary diffusion coefficients of species  $i$  with respect to nitrogen is approximately proportional to

$$D_i \sim \left( \frac{W_i + W_{N_2}}{2W_i W_{N_2}} \right)^{1/2}$$

Then the ratio of its Lewis number to that of methane is

$$\frac{Le_i}{Le_{CH_4}} = \left( \frac{W_i}{W_{CH_4}} \frac{W_{CH_4} + W_{N_2}}{W_i + W_{N_2}} \right)^{1/2}$$



## Balance Equations for Element Mass Fractions

Summation of the balance equations for the mass fractions

$$\rho \frac{DY_i}{Dt} = -\mathbf{div} \mathbf{j}_i + \dot{m}_i, \quad i = 1, 2, \dots, k.$$

according to

$$Z_j = \frac{m_j}{m} = \sum_{i=1}^k \frac{a_{ij} W_j}{W_i} Y_i = \frac{W_j}{W} \sum_{i=1}^k a_{ij} X_i, \quad j = 1, 2, \dots, k_e,$$

leads to the balance equations for  $Z_j$ :  $\rho \frac{DZ_j}{Dt} = -\mathbf{div} \sum_{i=1}^k \frac{a_{ij} W_j}{W_i} \mathbf{j}_i$ .

Here the summation over the chemical source terms vanishes

$$W_j \sum_{i=1}^k \sum_{l=1}^r a_{ij} \nu_{il} w_l = W_j \sum_{l=1}^r w_l \sum_{i=1}^k a_{ij} \nu_{il} = 0$$

since the last sum vanishes for each reaction.

The diffusion term simplifies if one assumes that the diffusion coefficients of all species are equal.

If one further more assumes  $Le_i=1$  this leads to

$$\rho \frac{DZ_j}{Dt} = \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Z_j \right).$$

A similar equation may be derived for the mixture fraction  $Z$ .

Since  $Z$  is defined according to  $Z = \frac{m_1}{m_1 + m_2}$

as the mass fraction of the fuel stream, it represents the sum of element mass fractions contained in the fuel stream.

The mass fraction of the fuel is the sum of the element mass fractions

$$Y_{F,u} = \sum_{j=1}^{k_e} Z_{j,F},$$

where

$$Z_{j,F} = a_{F,j} \frac{W_j}{W_F} Y_{F,u}.$$

With  $Y_{F,u} = Y_{F,1}Z$  the mixture fraction may therefore be expressed as a sum of element mass fractions

$$Z = \frac{\sum_{j=1}^{k_e} Z_{j,F}}{Y_{F,1}}$$

Then, with the assumption of  $Le_i=1$ , a summation over

$$\rho \frac{DZ_j}{Dt} = \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Z_j \right)$$

leads to a balance equation for the mixture fraction

$$\rho \frac{DZ}{Dt} = \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Z \right).$$

For a one-step reaction with the reaction rate  $\omega$  this equation can also be derived using

$$Z = \frac{\nu Y_F - Y_{O_2} + Y_{O_2,2}}{\nu Y_{F,1} + Y_{O_2,2}}$$

and

$$\rho \frac{DY_i}{Dt} = \frac{1}{Le_i} \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Y_i \right) + W_i \sum_{l=1}^r \nu_{il} \omega_l$$

for  $Y_F$  and  $Y_{O_2}$  with  $Le_F = Le_{O_2} = 1$  as

$$\rho \frac{DY_F}{Dt} = \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Y_F \right) - \nu'_F W_F \omega$$

$$\rho \frac{DY_{O_2}}{Dt} = \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Y_{O_2} \right) - \nu'_{O_2} W_{O_2} \omega.$$

Dividing the first of these by  $\nu'_{\text{O}_2} W_{\text{O}_2}$  and subtracting yields a source-free balance equation for the combination

$$\frac{Y_{\text{F}}}{\nu'_{\text{F}} W_{\text{F}}} = \frac{Y_{\text{O}_2}}{\nu'_{\text{O}_2} W_{\text{O}_2}}$$

which is a linear function of  $Z$  according to

$$Z = \frac{m_1}{m_1 + m_2}$$

This leads again to

$$\rho \frac{\text{D}Z}{\text{D}t} = \text{div} \left( \frac{\lambda}{c_p} \text{grad } Z \right).$$

For constant pressure the enthalpy equation

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} h \right).$$

has the same form as

$$\rho \frac{DZ}{Dt} = \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Z \right).$$

and a coupling relation between the enthalpy and the mixture fraction may be derived

$$h = h_2 + Z(h_1 - h_2)$$

where  $h_1$  is the enthalpy of the fuel stream and  $h_2$  that of the oxidizer stream.

Similarly, using

$$\rho \frac{DZ_j}{Dt} = \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Z_j \right)$$

and

$$\rho \frac{DZ}{Dt} = \mathbf{div} \left( \frac{\lambda}{c_p} \mathbf{grad} Z \right).$$

the element mass fractions may be expressed in terms of the mixture fraction

$$Z_j = Z_{j,2} + Z(Z_{j,1} - Z_{j,2}),$$

where  $Z_{j,1}$  and  $Z_{j,2}$  are the element mass fractions in the fuel and oxidizer stream.



It should be noted that the coupling relations

$$h = h_2 + Z(h_1 - h_2)$$

and

$$Z_j = Z_{j,2} + Z(Z_{j,1} - Z_{j,2})$$

required a **two feed system** with equivalent boundary conditions for the enthalpy and the mass fractions.

A practical example is a single jet as fuel stream with co-flowing air as oxidizer stream into an open atmosphere, such that zero gradient boundary conditions apply everywhere except at the input streams.

Once the mixture fraction field has been obtained by numerical solution of

$$\rho \frac{DZ}{Dt} = \text{div} \left( \frac{\lambda}{c_p} \text{grad } Z \right)$$

the adiabatic flame temperature may be calculated using the methods of lecture 2 as a local function of  $Z$ .

