

Fluid Dynamics and Balance Equations for Reacting Flows

Combustion Summer School

2018

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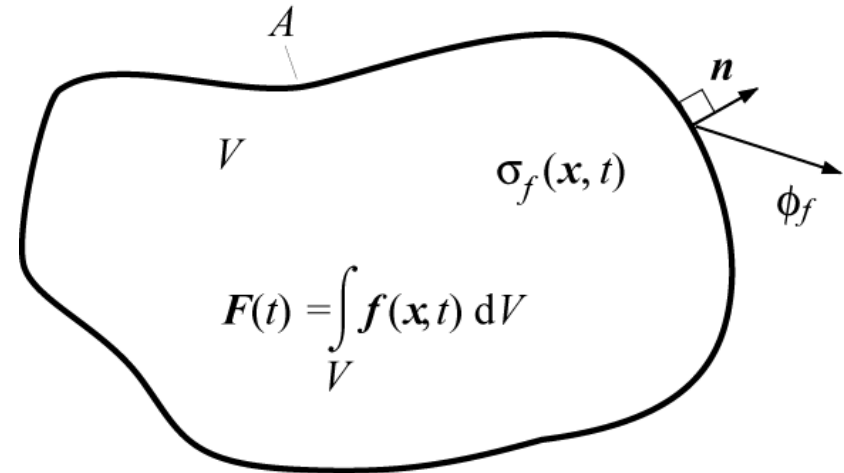


Balance Equations

- 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 ϕ_f and the normal vector n determines the outflow through the surface A , a source s_f the rate of production of $F(t)$
- Let us consider a general quantity per unit volume $f(\mathbf{x}, t)$. Its integral over the finite volume V , with the time-independent boundary A is given by



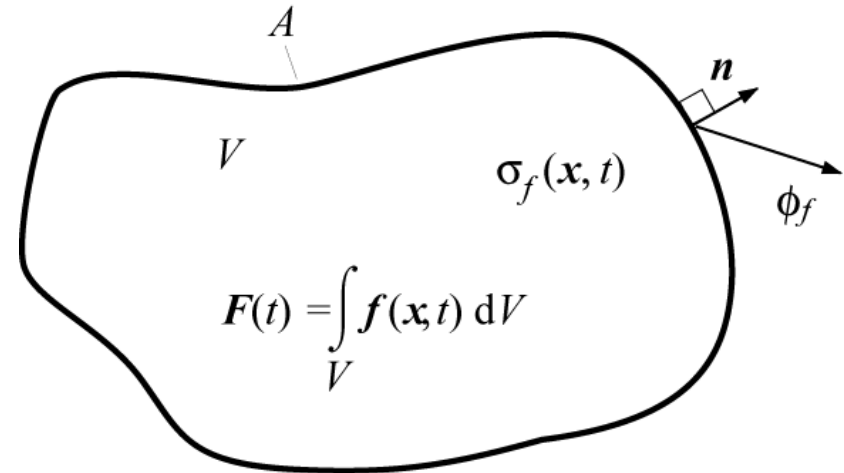
$$F(t) = \int_V f(\mathbf{x}, t) dV$$

Balance Equations

- 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 \mathbf{f}_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

$$- \int_A \phi_f \cdot \mathbf{n} dA,$$

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

Balance Equations

- 2. by a local source \mathbf{s}_f within the volume.

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

Integrating the source term over the volume leads to

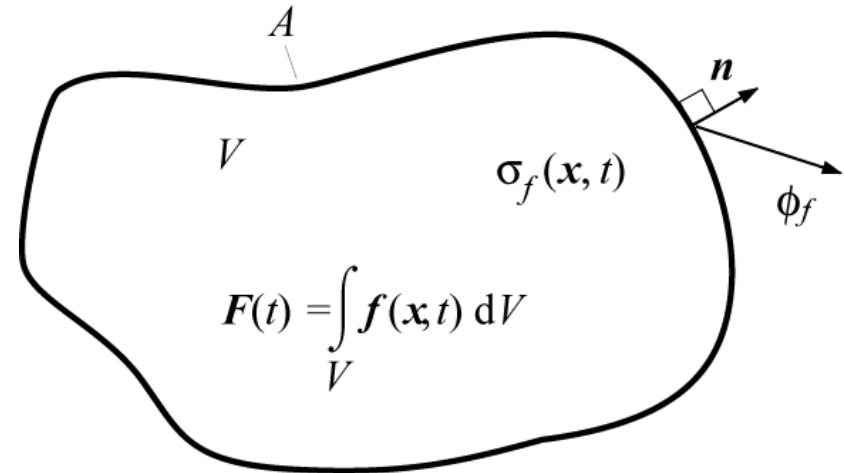
$$\int_V \sigma_f dV$$

- 3. by an external induced source \mathbf{s} .

Examples are the gravitational force or thermal radiation.

Integration of \mathbf{s}_f over the volume yields

$$\int_V \mathbf{s}_f dV$$



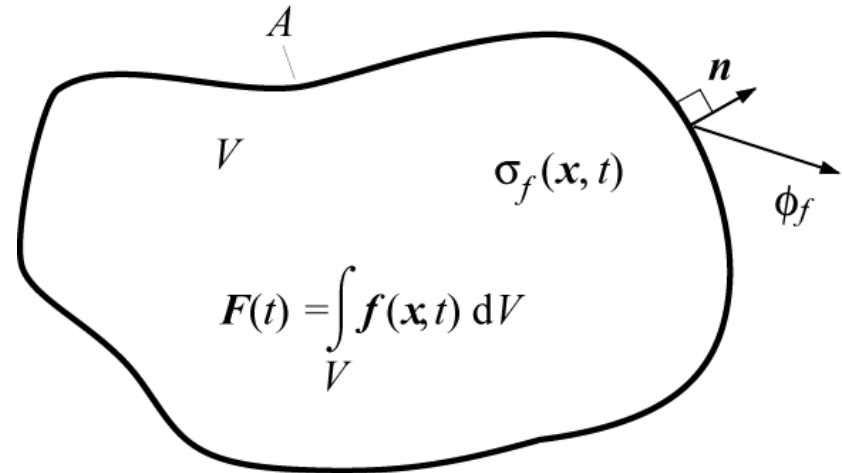
Balance Equations

- We therefore have the balance equation

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

- Changing the integral over the boundary A
Gauss' theorem

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

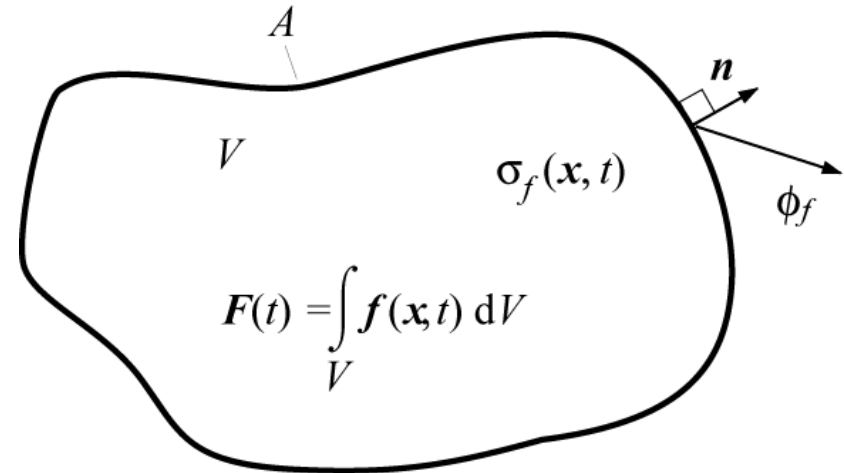


and realizing that the balance must be independent of the volume, we obtain the general balance equation in differential form

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

Mass Balance

- Set the partial mass per unit volume $\rho_i = \rho Y_i = f$.
- The partial mass flux across the boundary is $\rho_i \mathbf{v}_i = \phi_f$, where \mathbf{v}_i is called the diffusion velocity.



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

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

$$\sum_{i=1}^k \mathbf{j}_i = \mathbf{0}.$$

Mass Balance

- 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](#)

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

Mass Balance

- 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 $\rho \mathbf{v} = \mathbf{f}$.
- The momentum flux is the sum of the convective momentum in flow $\rho \mathbf{v} \mathbf{v}$ and the stress tensor

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

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

- Therefore $\rho \mathbf{v} \cdot \mathbf{v} + \mathbf{P} = \boldsymbol{\phi}_f$.
- There is no local source of momentum, but the gravitational force from outside

$$s_f = \rho \mathbf{g}$$

where \mathbf{g} denotes the constant of gravity.

Momentum Balance

- 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

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

with v provides the balance for the kinetic energy

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

where $v^2 = \mathbf{v} \cdot \mathbf{v}$.

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

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

- 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

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

Total and Internal Energy and Enthalpy Balance

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

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

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

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

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

- Here the suffix ^{sym} 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**.

Transport Processes

- 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

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

- 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**.

Transport Processes

- 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

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

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

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

Transport Processes

- Note that the use of $\mathbf{j}_i = -\rho D_i \mathbf{grad} Y_i$, $D_i = D_{i,N_2}$

$$\sum_{i=1}^k \mathbf{j}_i = \mathbf{0}.$$

does not satisfy the condition

- 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** λ .

Transport Processes

- 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

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

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.

Different Forms of the Energy Equation

- We can write the heat flux as

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

- If the diffusion flux can be approximated by

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

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

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

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

Different Forms of the Energy Equation

- 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.

Different Forms of the Energy Equation

- 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

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

Different Forms of the Energy Equation

- Then with

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

the enthalpy equation

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

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.

Different Forms of the Energy Equation

- 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.

Different Forms of the Energy Equation

- 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

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

Different Forms of the Energy Equation

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

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

H ₂	CO	H ₂ O ₂	HCO	CH ₂ O	CH ₃	CH ₃ 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
$$\rho \frac{DT}{Dt} = \frac{1}{c_p} \frac{Dp}{Dt} + \text{div} \left(\frac{\lambda}{c_p} \mathbf{grad} T \right) + \sum_{l=1}^r \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p}$$

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

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

Different Forms of the Energy Equation

- 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 $\text{Pr} = \frac{\mu c_p}{\lambda} = 0.75,$

and constant Lewis numbers $\text{Le}_i = \frac{\lambda}{\rho c_p D_i}$

Different Forms of the Energy Equation

- 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.

Balance Equations for Element Mass Fractions

- 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

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

Balance Equations for Element Mass Fractions

- 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

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

Balance Equations for Element Mass Fractions

- 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 $Le_j=1$, 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

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

Balance Equations for Element Mass Fractions

- For a one-step reaction with the reaction rate w 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

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

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

Balance Equations for Element Mass Fractions

- Dividing the first of these by $\nu'_{O_2} W_{O_2}$ and subtracting yields a source-free balance equation for the combination

$$\frac{Y_F}{\nu'_F W_F} = \frac{Y_{O_2}}{\nu'_{O_2} W_{O_2}}$$

which is a linear function of Z according to

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

- This leads again to

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

Balance Equations for Element Mass Fractions

- 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.

Balance Equations for Element Mass Fractions

- 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.

Balance Equations for Element Mass Fractions

- 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.

Balance Equations for Element 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

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

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

