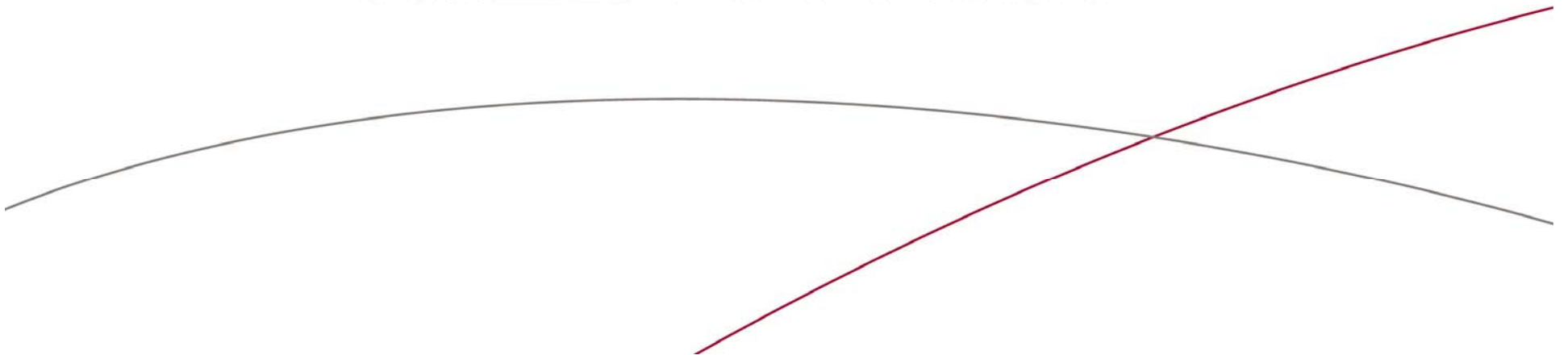




## Lecture 4

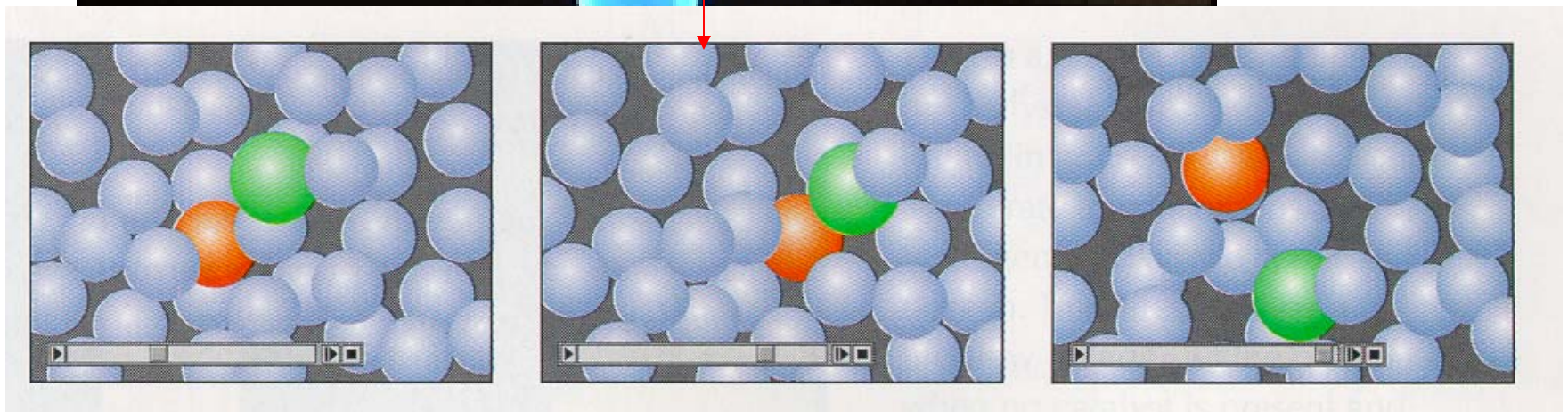
# Transport of mass, momentum and heat



# Flow and molecular motion



turbulent jet  
flame



# Mean speed of molecules: microscopic scale

$$s_i = \left( \frac{8k_B T}{\pi m_i} \right)^{1/2}$$

$k_B$  is Boltzmann's constant,  $m_i$  is the mass of molecule  $i$ .

# Mean speed of molecules: microscopic scale

$$\vec{v} = \frac{\sum_{i=1}^N \rho_i \vec{v}_i}{\sum_{i=1}^N \rho_i} = \frac{\sum_{i=1}^N \rho_i \vec{v}_i}{\rho} = \sum_{i=1}^N Y_i \vec{v}_i$$

Define a mass averaged mean velocity

# Mass transfer

- A mixture containing N species, each species has different velocity

$$\vec{v}_i = \vec{v} + \vec{V}_i$$

Velocity of species  $i$

Mass averages velocity of mixture

Diffusion velocity of species  $i$

$$\vec{v} = \sum_{i=1}^N Y_i \vec{v}_i$$
$$\sum_{i=1}^N Y_i \vec{V}_i = 0$$



# Mass transfer

# Mass transfer

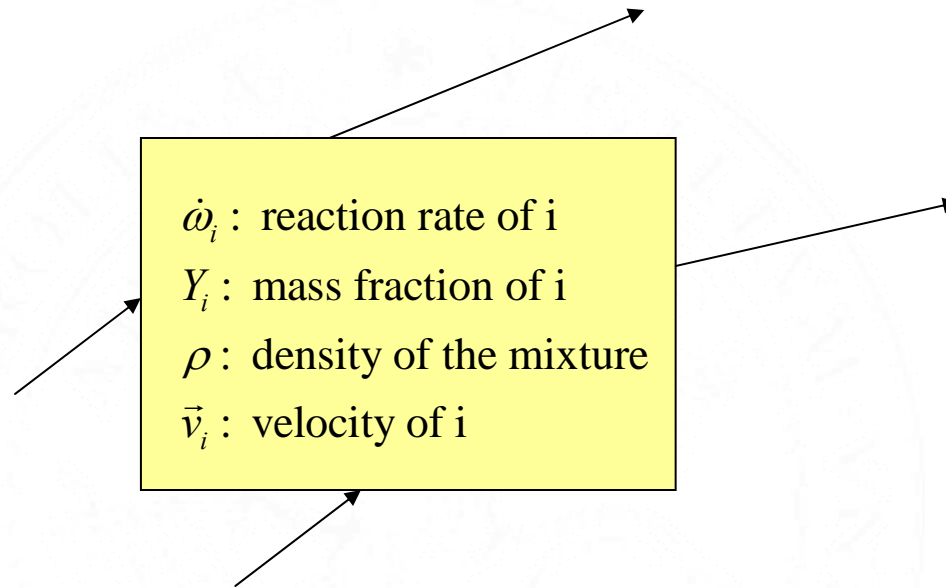
- $\vec{V}_i$ 
  - diffusion velocity due to concentration gradient
  - diffusion velo. due to temperature gradient (Soret)
  - diffusion velocity due to pressure gradient
- the last two effects can be neglected
- diffusion by concentration gradient is modeled by Fick's Law

$$Y_i \vec{V}_i = -D_{iN} \nabla Y_i$$

Negative sign indicate flux from high concentration to low

Binary diffusivity

# A control volume CV for mass conservation



A control volume CV for mass conservation: the boundary is open, species can enter or leave the CV; it can also be formed or consumed in the CV



# Law of mass conservation

Law of mass conservation says that *the increase of the total mass of species  $i$  in the CV is equal to the net mass flow into the CV + the formation rate of the species in the CV.*

# Mass transfer

- Transport of species  $i$  in a mixture of  $N$  species, in a control volume ...

Change of mass of species  $i$  = Net mass flux in + Formation rate of species  $i$

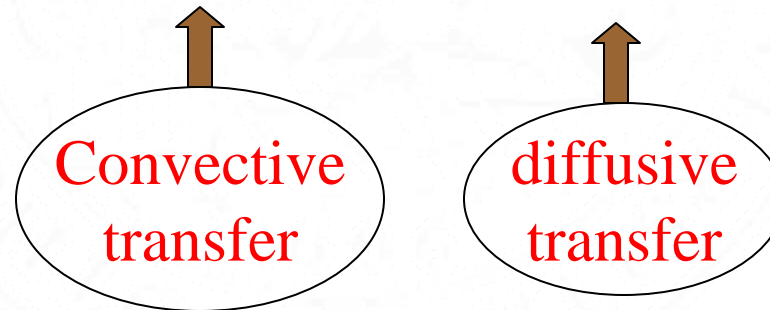
$$\frac{\partial \rho Y_i}{\partial t} = -\nabla \cdot \rho Y_i \vec{v}_i + \omega_i$$

Known from chemical kinetics

# Mass transfer

- Using Fick's Law one has the transport equation for species  $i$
- This equation is not closed without reaction kinetics rate information !

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \rho Y_i \vec{v} = \nabla \cdot \rho D_{iN} \nabla Y_i + \omega_i$$



# Mass transfer

- Summation over all species we have

$$\frac{\partial \rho \sum_{i=1}^N Y_i}{\partial t} = -\nabla \cdot \rho \sum_{i=1}^N Y_i \vec{v} + \sum_{i=1}^N \omega_i$$

**=1** (pointing to the summation  $\sum_{i=1}^N Y_i$ )

**=0** (pointing to the summation  $\sum_{i=1}^N \omega_i$ )

**Law of mass action** (circled text with an arrow pointing to the summation  $\sum_{i=1}^N \omega_i$ )

**Hi, I know it !  
It's the continuity equation !** (starburst callout)

**⇒**  $\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v} = 0$



# Momentum conservation

# Momentum conservation

We consider the momentum conservation of the mixture.

The law of momentum conservation is the Newton's second law applied to Fluid Mechanics, which states that *the change of the total momentum in the CV (Fig.4.1) + the exchange of momentum through the boundary of the CV is equal to the forces acting on the boundary + the body forces on the CV.*

# Momentum transfer

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot \rho \vec{v} \vec{v} = \nabla \cdot (pI + \tau), \text{ or } \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (i = 1, 2, 3)$$

$$\text{or } \rho \frac{\partial \vec{v}}{\partial t} + \rho \vec{v} \cdot \nabla \vec{v} = \nabla \cdot (pI + \tau), \text{ or } \rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

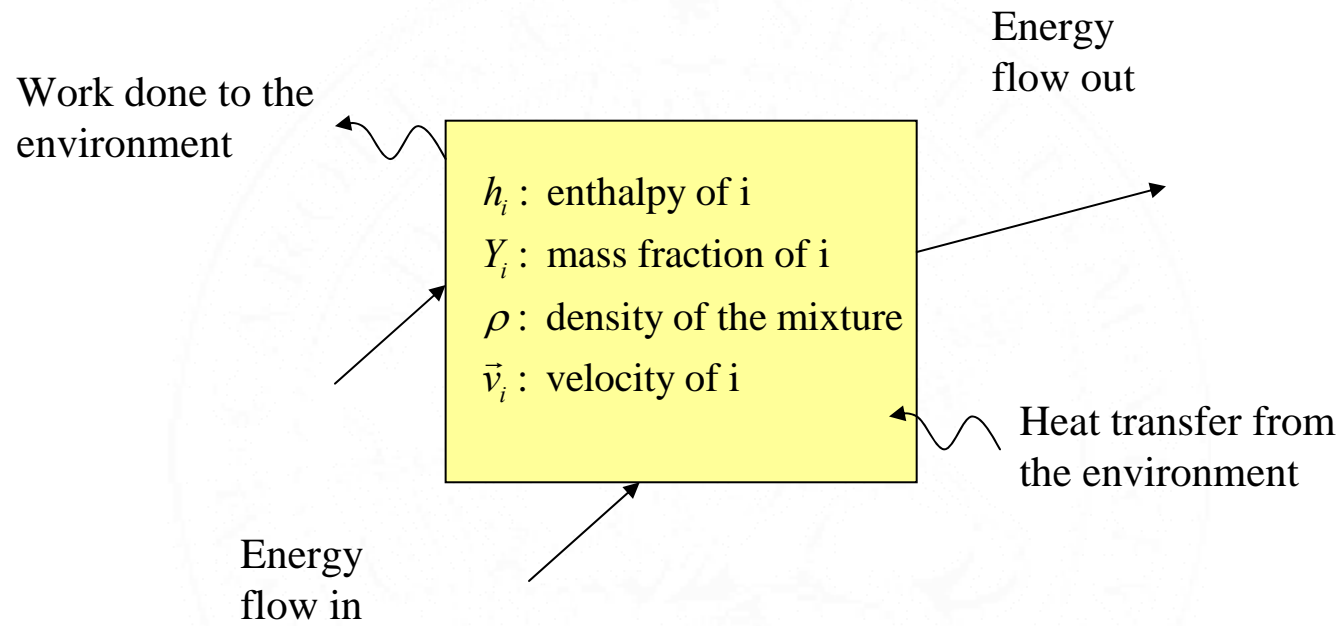
$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \mu \frac{\partial u_k}{\partial x_k}$$



# Energy conservation



# A control volume CV for energy conservation



the boundary is open, species can enter or leave the CV;  
it can also be formed or consumed in the CV

# Total energy change per unit mass

$$\begin{aligned}e_{total} &= e + \frac{1}{2}v^2 \\&= \sum_{i=1}^N Y_i e_i + \frac{1}{2}v^2 \\&= \sum_{i=1}^N Y_i h_i - \frac{p}{\rho} + \frac{1}{2}v^2 \\&= \left( h - \frac{p}{\rho} \right) + \frac{1}{2}v^2\end{aligned}$$

# The energy flux at an open boundary

- Energy flux due to mass flow of species through the CV boundaries
- Energy flux due to temperature gradient through the CV boundaries
- Energy flux due to concentration gradient at the boundaries (Dufour effect, often negligible)

# Energy flux due to flow motion

$$\begin{aligned}\sum_{i=1}^N \rho_i \vec{v}_i \left( e_i + \frac{1}{2} v^2 \right) &= \sum_{i=1}^N \rho Y_i (\vec{v} + \vec{V}_i) \left( h_i - \frac{p}{\rho} + \frac{1}{2} v^2 \right) \\ &= \rho \vec{v} \sum_{i=1}^N Y_i \left( h_i - \frac{p}{\rho} + \frac{1}{2} v^2 \right) + \rho \sum_{i=1}^N Y_i \vec{V}_i \left( h_i - \frac{p}{\rho} + \frac{1}{2} v^2 \right) \\ &= \rho \vec{v} \sum_{i=1}^N Y_i h_i + \rho \vec{v} \sum_{i=1}^N Y_i \left( -\frac{p}{\rho} + \frac{1}{2} v^2 \right) + \rho \sum_{i=1}^N Y_i \vec{V}_i h_i + \rho \sum_{i=1}^N Y_i \vec{V}_i \left( -\frac{p}{\rho} + \frac{1}{2} v^2 \right) \\ &= \rho \vec{v} h + \rho \vec{v} \left( -\frac{p}{\rho} + \frac{1}{2} v^2 \right) + \rho \sum_{i=1}^N Y_i \vec{V}_i h_i\end{aligned}$$

# Energy flux due to temperature gradients

$$\vec{q} = -\lambda \nabla T$$



heat conductivity

# Total energy flux

- Through the boundary of a control volume

$$\vec{q}_{total} = \vec{q} + \rho \vec{v} h + \rho \vec{v} \left( -\frac{p}{\rho} + \frac{1}{2} v^2 \right) + \rho \sum_{i=1}^N Y_i \vec{V}_i h_i$$

$\uparrow$  conduction                      convection                       $\uparrow$  diffusion

# work per unit area done to the environment

$$\left(-pI + \tau\right) \cdot \vec{v}$$

# First law of thermodynamics

The first law of thermodynamics states that the energy increase in a system is equal to the heat transfer from the environment to the system - work done to the system. In differential equation form one can write

$$\frac{\partial}{\partial t}(\rho e_{total}) + \nabla \cdot \vec{q}_{total} = \dot{Q}_r + \nabla \cdot [(-pI + \tau) \cdot \vec{v}]$$



# Energy transport equation – conventional forms

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \rho h - p + \frac{1}{2} \rho v^2 \right) \\ & + \nabla \cdot \left( \vec{q} + \rho \vec{v} h + \vec{v} \left( -p + \rho \frac{1}{2} v^2 \right) + \rho \sum_{i=1}^N Y_i \vec{V}_i h_i \right) \\ & = \dot{Q}_r + \nabla \cdot [(-pI + \tau) \cdot \vec{v}] \end{aligned}$$

# Energy transport equation – conventional forms

$$\vec{v} \cdot \left( \rho \frac{\partial \vec{v}}{\partial t} + \rho \vec{v} \cdot \nabla \vec{v} \right) = \vec{v} \cdot (\nabla \cdot (-pI + \tau))$$

$$\Rightarrow \rho \frac{\partial \frac{1}{2} v^2}{\partial t} + \rho \vec{v} \cdot \nabla \frac{1}{2} v^2 = \nabla \cdot [(-pI + \tau) \cdot \vec{v}] - (-pI + \tau) : \nabla \vec{v}$$

$$\Rightarrow \frac{\partial \frac{1}{2} \rho v^2}{\partial t} + \nabla \cdot \left( \frac{1}{2} \rho \vec{v} v^2 \right) = \nabla \cdot [(-pI + \tau) \cdot \vec{v}] - (-pI + \tau) : \nabla \vec{v}$$

# Energy transport equation – conventional forms

$$\frac{\partial}{\partial t}(\rho h - p) + \nabla \cdot \left( \vec{q} + \rho \vec{v} h + \vec{v}(-p) + \rho \sum_{i=1}^N Y_i \vec{V}_i h_i \right) \\ = \dot{Q}_r + (-pI + \tau) : \nabla \vec{v}$$

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla \equiv \frac{\partial}{\partial t} + u_j \frac{\partial}{\partial x_j}$$

$$\rho \frac{Dh}{Dt} - \frac{Dp}{Dt} = -\nabla \cdot \left( \vec{q} + \rho \sum_{i=1}^N Y_i \vec{V}_i h_i \right) + \dot{Q}_r + \tau : \nabla \vec{v}$$

# Energy transport equation – conventional forms

$$\rho \frac{Dh}{Dt} - \frac{Dp}{Dt} = \nabla \cdot \left( \rho \alpha \nabla h - \rho \alpha \sum_{i=1}^N \left( 1 - \frac{1}{Le_i} \right) h_i \nabla Y_i \right) + \dot{Q}_r + \tau : \nabla \vec{v}$$

Lewis number

$$Le_i \equiv \frac{\alpha}{D_i} = \frac{\lambda}{\rho c_p D_i}$$

# Energy transport equation – conventional forms

$$\rho \frac{Dh}{Dt} - \frac{Dp}{Dt} = \nabla \cdot \left( \rho \alpha \nabla h - \rho \alpha \sum_{i=1}^N \left( 1 - \frac{1}{Le_i} \right) h_i \nabla Y_i \right) + \dot{Q}_r + \tau : \nabla \vec{v}$$



$$\rho \frac{Dh}{Dt} = \nabla \cdot (\rho \alpha \nabla h)$$

# Energy transport equation – conventional forms

$$\begin{aligned} & \rho c_p \frac{DT}{Dt} - \frac{Dp}{Dt} \\ &= \nabla \cdot (\lambda \nabla T) + \sum_{i=1}^N (\rho D_i c_{pi} \nabla Y_i \cdot \nabla T) - \dot{\omega}_i h_i + \dot{Q}_r + \tau : \nabla \vec{v} \\ & \quad \downarrow \\ & \rho c_p \frac{DT}{Dt} = \nabla \cdot (\lambda \nabla T) + \sum_{i=1}^N (\rho D_i c_{pi} \nabla Y_i \cdot \nabla T) - \dot{\omega}_i h_i \end{aligned}$$

# Energy transfer

- in species transport equations, there is a source term due to chemical reaction, why there is no source term due to chemical reactions in the energy equation?
- chemical energy is released to thermal energy, however the system's energy is not changed due to chemical reactions !
- If energy equation is expressed as temperature transport equation, one should have the reaction source term

# Summary of governing equations

- Unknowns
  - 3 velocity components
  - pressure
  - temperature or enthalpy
  - N species
  - density
- total unknowns
  - $N+6$
- Governing equations
  - continuity 1
  - N-S equations 3
  - temperature or enthalpy 1
  - equation of state 1
  - species transport N
- total equations
  - $N+6$



# Simplified governing equations (unity Lewis number)

Mass: 
$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0$$

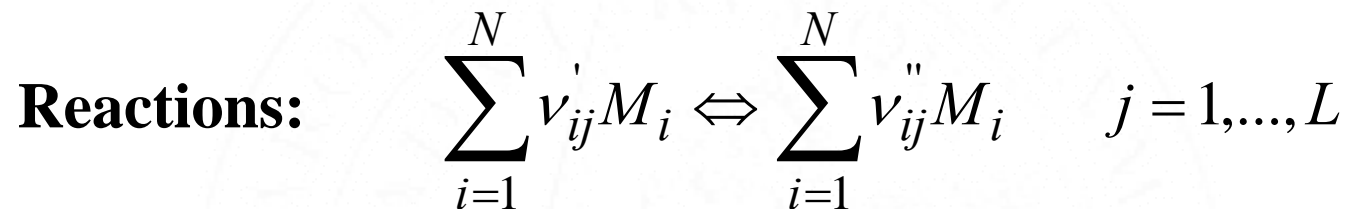
Momentum: 
$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

Energy: 
$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_i h}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{\text{Pr}} \frac{\partial h}{\partial x_j} \right) + \dot{Q}_r$$

Species: 
$$\frac{\partial \rho Y_i}{\partial t} + \frac{\partial \rho u_j Y_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{\text{Sc}} \frac{\partial Y_i}{\partial x_j} \right) + \omega_i$$

Equation of state: 
$$p = R_0 \rho T \sum_i \frac{Y_i}{W_i}$$

# Chemical reaction rates



**Reaction rates:**

$$\omega_i \equiv \frac{dC_i}{dt} = \sum_{j=1}^L (\nu''_{ij} - \nu'_{ij}) q_j$$

$$q_j = k_{jf} \prod_{i=1}^N C_i^{\nu'_{ij}} - k_{jb} \prod_{i=1}^N C_i^{\nu''_{ij}}$$

# A comparison of mass diffusivity, heat conductivity and viscosity

Using kinetic theory it can be shown (cf. Turns book):

$$D_{ij} = \frac{1}{3} c \xi = \frac{2}{3} \left( \frac{k_B^3 T}{\pi^3 m_{ij}} \right)^{1/2} \frac{T}{\sigma^2 P} \propto T^{3/2} P^{-1}$$

Mean diffusion coefficient for species  $i$  in the mixture

$$D_i = \frac{1 - Y_i}{\sum_{j=1, j \neq i}^N X_j / D_{ij}} \propto T^{3/2} P^{-1}$$

# A comparison of mass diffusivity, heat conductivity and viscosity

Using kinetic theory it can be shown (cf. Turns book):

$$k = \frac{1}{2} k_B \left( \frac{n}{V} \right) c_{\xi} = \left( \frac{k_B^3 T}{\pi^3 m \sigma^4} \right)^{1/2} \propto T^{1/2}$$

Thermal diffusion coefficient  $\alpha \equiv \frac{k}{\rho c_p}$

Lewis number  $Le_i \equiv \frac{k}{\rho c_p D_i} = \frac{\alpha}{D_i}, \quad \therefore D_i = \frac{\alpha}{Le_i}$

# A comparison of mass diffusivity, heat conductivity and viscosity

Using kinetic theory it can be shown:

$$\mu = \frac{1}{3} \rho c \xi = \frac{2}{3} \left( \frac{m k_B T}{\pi^3 \sigma^4} \right)^{1/2} \propto T^{1/2}$$

Prandtl number

$$\text{Pr} \equiv \frac{\mu}{\rho \alpha} = \frac{\nu}{\alpha}$$

Schmidt number

$$\text{Sc}_i \equiv \frac{\mu}{D_i}$$