

# Class 19 - Conservation Eqns, Shuvalov - Zeldovich

• Detailed Derivations included

## Summary

$$\text{Mass: } \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{v})$$

$$\text{Species: } \frac{\partial \rho Y_i}{\partial t} = -\nabla \cdot (\rho \vec{v} Y_i) - \nabla \cdot (\vec{j}_i) + \omega_i \Gamma_i$$

$$\text{Momentum: } \frac{\partial \rho \vec{v}}{\partial t} = -\nabla \cdot (\rho \vec{v} \vec{v}) - \nabla \cdot (\underline{\underline{\tau}}) - \nabla(P) + \rho \vec{g}$$

$$\text{Energy: } \frac{\partial \rho e}{\partial t} = -\nabla \cdot (\rho \vec{v} e) - \nabla \cdot (\vec{q}) - \nabla \cdot (\underline{\underline{\tau}} \cdot \vec{v}) - \nabla \cdot (P \vec{v}) + \rho \vec{g} \cdot \vec{v}$$

(Accum)      (Convection)      (Diffusion)      (Source/Work)

$-\nabla \cdot \text{flux}$

$\rho \vec{v} (=)$	$\frac{\text{kg}}{\text{m}^2 \cdot \text{s}}$	mass
$\rho \vec{v} Y_i (=)$	$\frac{\text{kg}_i}{\text{m}^2 \cdot \text{s}}$	species
$\rho \vec{v} \vec{v} (=)$	$\frac{\text{kg} \cdot \text{m/s}}{\text{m}^2 \cdot \text{s}}$	mom
$\rho \vec{v} e (=)$	$\frac{\text{J}}{\text{m}^2 \cdot \text{s}}$	energy

$$-\nabla \cdot \text{flux} \equiv (\text{in}) - (\text{out})$$



$$\int_{CV} -\nabla \cdot \vec{f} dV = -\int_{CS} \vec{f} \cdot \vec{n} dA = -[f_{out} \cdot A - f_{in} \cdot A]$$

$$= (f_{in} A) - (f_{out} A)$$

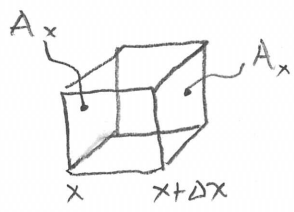
Vars

Mass	:	$\rho$	} Governing Eqns
Species	:	$Y_i$	
Momentum	:	$\vec{v}$	
Energy	:	$e$	
<hr/> $P = \rho RT/M$			} Equation of State.
$f_i = f_i(T, P, Y_i)$			} Constitutive Relations: $f_i, q, \tau$ (Source Term $w_i$ )
$\omega_i = \omega_i(T, P, Y_i)$			
$\tau_i = \tau_i(T, P, Y_i, \vec{v})$			
$q_i = q_i(T, P, Y_i, f_i)$			
<hr/> $T = T(Y_i, P, h)$			} Thermodynamic Relations
$h = e - \frac{1}{2} \vec{v} \cdot \vec{v} + \frac{P}{\rho}$			

• with  $C_p, D, \mu, \alpha, \chi_i, M_i, \text{ etc.}$

Derive

Species: Differential



Accum = in - out + gen

$$\frac{\partial m_i}{\partial t} = A_x (\rho Y_i v_x)_x - A_x (\rho Y_i v_x)_{x+\Delta x} + [Y_i, Z, \text{Divs}] + \omega_i M_i V_x$$

$$m_i = \rho Y_i V_x = \rho Y_i \Delta x \Delta y \Delta z$$

$$A_x = \Delta y \Delta z$$

$$\div \Delta x \Delta y \Delta z$$

$$\frac{\partial \rho Y_i}{\partial t} = \frac{(\rho Y_i v_x)_x - (\rho Y_i v_x)_{x+\Delta x}}{\Delta x} + \frac{[Y_i, Z - \text{Divs}]}{\Delta y, \Delta z} + \omega_i M_i$$

$$\lim_{\Delta x \rightarrow 0} \left[ \frac{(\rho Y_i v_x)_x - (\rho Y_i v_x)_{x+\Delta x}}{\Delta x} \right] = -\nabla \cdot (\rho Y_i v_x)$$

$$V_a = V + V_a^D \rightarrow \rho Y_i V_a = \rho Y_i V + \rho Y_i V_a^D = \rho Y_i V + \tau_i$$

Species: integral.

$$RTT: \frac{dB}{dt} = \frac{\partial}{\partial t} \int_{CV} \rho b dV + \int_{CS} \rho b \vec{V}_r \cdot \vec{n} dA$$

$$\bullet B = m_i, \quad b = B/m = Y_i \quad \bullet \vec{V}_r = \vec{V}_i = \vec{V} + V_i^D$$

$$\bullet \frac{dB}{dt} = \frac{dm_i}{dt} = \int_{CV} M_i \omega_i dV$$

$$\int_{CV} M_i \omega_i dV = \frac{\partial}{\partial t} \int_{CV} \rho Y_i dV + \int_{CS} \rho Y_i \vec{V}_i \cdot \vec{n} dA$$

$$\int_{CV} \nabla \cdot (\rho Y_i \vec{V}_i) dV$$

All terms  $\int_{CV} \cdot dV$

$$\rightarrow \frac{\partial \rho Y_i}{\partial t} = -\nabla \cdot (\rho Y_i \vec{V}_i) + \omega_i M_i$$

$$\rightarrow \frac{\partial \rho Y_i}{\partial t} = -\nabla \cdot (\rho Y_i \vec{V}) - \nabla \cdot \tau_i + \omega_i M_i$$

Coordinates

$\nabla \cdot$

Cartesian:  $\nabla \cdot \vec{f} = \frac{\partial f_x}{\partial x} + \frac{\partial f_y}{\partial y} + \frac{\partial f_z}{\partial z}$

Cylindrical:  $\nabla \cdot \vec{f} = \frac{1}{r} \frac{\partial}{\partial r} (r f_r) + \frac{1}{r} \frac{\partial f_\theta}{\partial \theta} + \frac{\partial f_z}{\partial z}$

$\nabla$

Cartesian  $\nabla f = \frac{\partial f}{\partial x} \vec{i} + \frac{\partial f}{\partial y} \vec{j} + \frac{\partial f}{\partial z} \vec{k}$

Cylindrical  $\nabla f = \frac{\partial f}{\partial r} \vec{r} + \frac{1}{r} \frac{\partial f}{\partial \theta} \vec{\theta} + \frac{\partial f}{\partial z} \vec{k}$

- Do a lot with Cylindrical,
- See BSL APP B, DGCAAT

# Sivbels - Zeldovich Formns.

- Simplify Eqns for Flame analysis.

\*  $\rho \vec{v} \cdot \nabla h_s - \nabla \cdot (\rho D \nabla h_s) = - \sum h_{f,c} \dot{m}_i'''$

•  $h_s = \int_{T_r}^T c_p dT$

• Turns (7.63 - 7.66.)

• Assumptions.

• S.S.

•  $Le_i = \frac{\alpha}{D_i} = \frac{\lambda}{\rho c_p D_i} = 1 \quad (D_i = \lambda / \rho c_p)$

• Fick's Law:  $\dot{J}_i = -\rho D_i \nabla Y_i$

• No P.E. (gravity)

• No shaft work, visc. Dissip.

• No radiation

• No K.E. (compared to  $\Delta H_{comb}$ )

• (No axial Diffusion B.L.A.)

B.L. Approx: (Axisymmetric  $\rightarrow$  Jets!)

• width small vs length

•  $\frac{\partial}{\partial r} \gg \frac{\partial}{\partial x}$

(neglect axial Diffusion)

•  $v_x \gg v_r$

- Mom

• species

• energy.

Energy

# Details: Conservation Laws

- Recap:
- Stoichiometry
  - Thermochemistry
  - Mass Transfer
  - Kinetics

\* Skip Section on Multicomponent Diffusion.  
Friday = Movie: Jetfire.

Basic Coupling - Flow/Chemistry - OD = PSR  
PFR/Batch

Flames require Spatial Conservation 1D - 3D.

↳ General Conservation Laws for Mass/Species, Momentum, Energy.

- General Conservation Laws: Mass, Mom, Energy
  - Cartesian
  - Cylindrical
  - Spherical
- Schweb-Zeldovich forms (Simplify)
- Conserved-Scalar Equation (Mixture fraction)

## Derive Conservation Laws

- Common: Balance on a C.V. Then shrink to Differential.
- Here: Start w/ R.T.T. Then apply Conservation Laws.
  - Integral form → Differential.

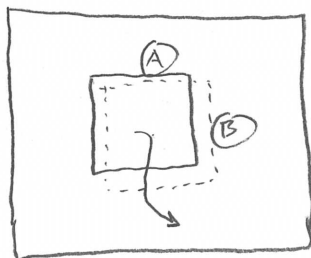
## Reynolds Transport Theorem (RTT)

Conservation Laws: "Mass is not created or Destroyed"  
 $dU = dQ + dW$   
 $F = ma$

These all apply to Lagrangian Systems (moving)

- we Define some Mass Then Describe Mass, mom, energy Conservation of That moving mass.
- There are not Control Volume analyses!
- Conservation Laws were not written for fixed Extension Control Volumes

\* The RTT Couples The Lagrangian System for which we have a Conservation law to The Eulerian Control Volumes Convenient for analysis



• Considers a System of fixed mass

- (A)
  - It moves in space
  - Its Shape / Volume Deforms
  - Lagrangian

• Considers a Control Volume (CV) That is fixed in space / shape.

- (B)
  - Eulerian

• At a given time, take The System and C.V. to overlap (but they only overlap for one instant)

- Let B be an extensive property of the system (Like Mass or Energy)

- Let b = B/mass

\* RTT  $\equiv$  "rate of change of B in the Lagrangian moving system = rate of change of B in the fixed Eulerian C.V. + rate at which B leaves that C.V."

$$\frac{dB}{dt} = \frac{d}{dt} \int_{CV} \rho b dV + \int_A \rho b \vec{v} \cdot \vec{n} dA \quad ; \quad \rho b \vec{v} \text{ is flux of } B$$

Lagrangian System

Eulerian CV

### Mass Conservation

• B = Mass, b = 1

• Conservation law  $\frac{dB}{dt} = \frac{dM}{dt} = 0$

$$\rightarrow 0 = \frac{d}{dt} \int_{CV} \rho dV + \int_A \rho \vec{v} \cdot \vec{n} dA$$

- Now pull  $\frac{d}{dt}$  inside  $\int$  (fixed C.V.)
  - Use Gauss Divergence Theorem:  $\int_A \vec{f} \cdot \vec{n} dA = \int_{CV} \nabla \cdot \vec{f} dV$
  - $0 = \int_{CV} \frac{\partial}{\partial t} \rho dV + \int_{CV} \nabla \cdot (\rho \vec{v}) dV$
  - $0 = \int_{CV} \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) \right] dV$
- $\rightarrow \boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0}$  Continuity equation.

Species Conservation

$B = M_i$ ;  $b = Y_i$

Conservation Law;  $\frac{dB}{dt} = \frac{dM_i}{dt} = \int_{CV} M_i \omega_i dV$

$\int_{CV} M_i \omega_i dV = \frac{d}{dt} \int \rho Y_i dV + \int_A \rho Y_i \vec{v}_i \cdot \vec{n} dA$   $\frac{kg}{m^2 s}$

or rearrange, apply G.D.T.

$\rightarrow \frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \vec{v}_i) = M_i \omega_i$

$v_i = v + v_i^D \rightarrow \rho Y_i v_i = \rho Y_i v + \rho Y_i v_i^D = \rho Y_i v + j_i$

\*  $\boxed{\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i v) = -\nabla \cdot j + M_i \omega_i}$

$j = -\rho D \nabla Y_i$

$\boxed{\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i v) = \nabla \cdot (\rho D \nabla Y_i) + M_i \omega_i}$

$= -\nabla \cdot j$

Momentum

$B = \text{Momentum} = m\vec{v}$  ;  $b = \vec{v}$

Conservation Law ;  $\frac{dm\vec{v}}{dt} = \sum \vec{F}_{\text{ext}}$  ( $F = ma = m\frac{dv}{dt} = \frac{dmv}{dt}$ )

- Pressure and viscous forces

$$\sum \vec{F}_{\text{ext}} = - \int_A (P\vec{e}_s + \underline{\underline{\tau}}) \cdot \vec{n} dA$$

$$- \int_A (P\vec{e}_s + \underline{\underline{\tau}}) \cdot \vec{n} dA = \frac{d}{dt} \int_{CV} \rho \vec{v} dV + \int_A \rho \vec{v} \vec{v} \cdot \vec{n} dA$$

Rearrange, use RTT

$$- \int_{CV} \nabla \cdot (P\vec{e}_s + \underline{\underline{\tau}}) dV = \frac{d}{dt} \int_{CV} \rho \vec{v} dV + \int_{CV} \nabla \cdot (\rho \vec{v} \vec{v}) dV$$

$$\rightarrow \frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot \rho \vec{v} \vec{v} = - \nabla \cdot \underline{\underline{\tau}} - \nabla \cdot P\vec{e}_s$$

$\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot \rho \vec{v} \vec{v} = - \nabla \cdot \underline{\underline{\tau}} - \nabla P$

 $+ \rho \vec{g}$

Energy

$B = E$  ;  $b = e = E/m$  ;  $e = \frac{1}{2}v^2 + u$  ;  $u = h - \frac{P}{\rho}$

Conservation Law:  $\frac{dE}{dt} = \dot{Q} + \dot{W} = - \int_A \vec{q} \cdot \vec{n} dA - \int_A \vec{F} \cdot \vec{v} dA + \int_{CV} \rho \vec{g} \cdot \vec{v} dV$

$\vec{F} = (P\vec{e}_s + \underline{\underline{\tau}}) \cdot \vec{n}$  (Dotting w/  $\vec{n}$  gives the force vector on the surface)

$$\frac{dE}{dt} = - \int_{CV} \nabla \cdot \vec{q} + \nabla \cdot (\underline{\underline{\tau}} \cdot \vec{v}) + \nabla \cdot (P\vec{e}_s \cdot \vec{v}) dV + \int_{CV} \rho \vec{g} \cdot \vec{v} dV$$

$$\rightarrow - \int_{CV} \nabla \cdot \vec{q} + \nabla \cdot (\underline{\underline{\tau}} \cdot \vec{v}) + \nabla \cdot P\vec{v} dV = \frac{d}{dt} \int_{CV} \rho e dV + \int_A \rho e \vec{v} \cdot \vec{n} dA$$

$\frac{dpe}{dt} + \nabla \cdot (pe\vec{v}) = - \nabla \cdot \vec{q} - \nabla \cdot (\underline{\underline{\tau}} \cdot \vec{v}) - \nabla \cdot P\vec{v} + \rho \vec{g} \cdot \vec{v}$



## The Fluxes and the Equations of Change

- §B.1 Newton's law of viscosity
- §B.2 Fourier's law of heat conduction
- §B.3 Fick's (first) law of binary diffusion
- §B.4 The equation of continuity
- §B.5 The equation of motion in terms of  $\tau$
- §B.6 The equation of motion for a Newtonian fluid with constant  $\rho$  and  $\mu$
- §B.7 The dissipation function  $\Phi_v$  for Newtonian fluids
- §B.8 The equation of energy in terms of  $q$
- §B.9 The equation of energy for pure Newtonian fluids with constant  $\rho$  and  $k$
- §B.10 The equation of continuity for species  $\alpha$  in terms of  $j_\alpha$
- §B.11 The equation of continuity for species  $A$  in terms of  $\omega_A$  for constant  $\rho_{AB}^0$

### §B.1 NEWTON'S LAW OF VISCOSITY

$$[\tau = -\mu(\nabla\mathbf{v} + (\nabla\mathbf{v})^\dagger) + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v})\delta]$$

Cartesian coordinates  $(x, y, z)$ :

$$\tau_{xx} = -\mu \left[ 2 \frac{\partial v_x}{\partial x} \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-1})^a$$

$$\tau_{yy} = -\mu \left[ 2 \frac{\partial v_y}{\partial y} \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-2})^a$$

$$\tau_{zz} = -\mu \left[ 2 \frac{\partial v_z}{\partial z} \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-3})^a$$

$$\tau_{xy} = \tau_{yx} = -\mu \left[ \frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y} \right] \quad (\text{B.1-4})$$

$$\tau_{yz} = \tau_{zy} = -\mu \left[ \frac{\partial v_z}{\partial y} + \frac{\partial v_y}{\partial z} \right] \quad (\text{B.1-5})$$

$$\tau_{zx} = \tau_{xz} = -\mu \left[ \frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x} \right] \quad (\text{B.1-6})$$

in which

$$(\nabla \cdot \mathbf{v}) = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \quad (\text{B.1-7})$$

<sup>a</sup> When the fluid is assumed to have constant density, the term containing  $(\nabla \cdot \mathbf{v})$  may be omitted. For monatomic gases at low density, the dilatational viscosity  $\kappa$  is zero.

## §B.1 NEWTON'S LAW OF VISCOSITY (continued)

Cylindrical coordinates ( $r, \theta, z$ ):

$$\tau_{rr} = -\mu \left[ 2 \frac{\partial v_r}{\partial r} \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-8})^a$$

$$\tau_{\theta\theta} = -\mu \left[ 2 \left( \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} \right) \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-9})^a$$

$$\tau_{zz} = -\mu \left[ 2 \frac{\partial v_z}{\partial z} \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-10})^a$$

$$\tau_{r\theta} = \tau_{\theta r} = -\mu \left[ r \frac{\partial}{\partial r} \left( \frac{v_\theta}{r} \right) + \frac{1}{r} \frac{\partial v_r}{\partial \theta} \right] \quad (\text{B.1-11})$$

$$\tau_{\theta z} = \tau_{z\theta} = -\mu \left[ \frac{1}{r} \frac{\partial v_z}{\partial \theta} + \frac{\partial v_\theta}{\partial z} \right] \quad (\text{B.1-12})$$

$$\tau_{zr} = \tau_{rz} = -\mu \left[ \frac{\partial v_r}{\partial z} + \frac{\partial v_z}{\partial r} \right] \quad (\text{B.1-13})$$

in which

$$(\nabla \cdot \mathbf{v}) = \frac{1}{r} \frac{\partial}{\partial r} (rv_r) + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z} \quad (\text{B.1-14})$$

<sup>a</sup> When the fluid is assumed to have constant density, the term containing  $(\nabla \cdot \mathbf{v})$  may be omitted. For monatomic gases at low density, the dilatational viscosity  $\kappa$  is zero.

Spherical coordinates ( $r, \theta, \phi$ ):

$$\tau_{rr} = -\mu \left[ 2 \frac{\partial v_r}{\partial r} \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-15})^a$$

$$\tau_{\theta\theta} = -\mu \left[ 2 \left( \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r}{r} \right) \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-16})^a$$

$$\tau_{\phi\phi} = -\mu \left[ 2 \left( \frac{1}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} + \frac{v_r + v_\theta \cot \theta}{r} \right) \right] + (\frac{2}{3}\mu - \kappa)(\nabla \cdot \mathbf{v}) \quad (\text{B.1-17})^a$$

$$\tau_{r\theta} = \tau_{\theta r} = -\mu \left[ r \frac{\partial}{\partial r} \left( \frac{v_\theta}{r} \right) + \frac{1}{r} \frac{\partial v_r}{\partial \theta} \right] \quad (\text{B.1-18})$$

$$\tau_{\theta\phi} = \tau_{\phi\theta} = -\mu \left[ \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \left( \frac{v_\phi}{\sin \theta} \right) + \frac{1}{r \sin \theta} \frac{\partial v_\theta}{\partial \phi} \right] \quad (\text{B.1-19})$$

$$\tau_{\phi r} = \tau_{r\phi} = -\mu \left[ \frac{1}{r \sin \theta} \frac{\partial v_r}{\partial \phi} + r \frac{\partial}{\partial r} \left( \frac{v_\phi}{r} \right) \right] \quad (\text{B.1-20})$$

in which

$$(\nabla \cdot \mathbf{v}) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 v_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (v_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} \quad (\text{B.1-21})$$

<sup>a</sup> When the fluid is assumed to have constant density, the term containing  $(\nabla \cdot \mathbf{v})$  may be omitted. For monatomic gases at low density, the dilatational viscosity  $\kappa$  is zero.

§B.2 FOURIER'S LAW OF HEAT CONDUCTION<sup>a</sup>

$$[\mathbf{q} = -k\nabla T]$$

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*Cartesian coordinates (x, y, z):*

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$$q_x = -k \frac{\partial T}{\partial x} \quad (\text{B.2-1})$$

$$q_y = -k \frac{\partial T}{\partial y} \quad (\text{B.2-2})$$

$$q_z = -k \frac{\partial T}{\partial z} \quad (\text{B.2-3})$$


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*Cylindrical coordinates (r, θ, z):*

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$$q_r = -k \frac{dT}{dr} \quad (\text{B.2-4})$$

$$q_\theta = -k \frac{1}{r} \frac{\partial T}{\partial \theta} \quad (\text{B.2-5})$$

$$q_z = -k \frac{\partial T}{\partial z} \quad (\text{B.2-6})$$


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*Spherical coordinates (r, θ, φ):*

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$$q_r = -k \frac{\partial T}{\partial r} \quad (\text{B.2-7})$$

$$q_\theta = -k \frac{1}{r} \frac{\partial T}{\partial \theta} \quad (\text{B.2-8})$$

$$q_\phi = -k \frac{1}{r \sin \theta} \frac{\partial T}{\partial \phi} \quad (\text{B.2-9})$$


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<sup>a</sup> For mixtures, the term  $\sum_\alpha (\bar{H}_\alpha / M_\alpha) \mathbf{j}_\alpha$  must be added to  $\mathbf{q}$  (see Eq. 19.3-3).

§B.3 FICK'S (FIRST) LAW OF BINARY DIFFUSION<sup>a</sup>

$$[j_A = -\rho \mathcal{D}_{AB} \nabla \omega_A]$$

Cartesian coordinates ( $x, y, z$ ):

$$j_{Ax} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial x} \quad (\text{B.3-1})$$

$$j_{Ay} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial y} \quad (\text{B.3-2})$$

$$j_{Az} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial z} \quad (\text{B.3-3})$$

Cylindrical coordinates ( $r, \theta, z$ ):

$$j_{Ar} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial r} \quad (\text{B.3-4})$$

$$j_{A\theta} = -\rho \mathcal{D}_{AB} \frac{1}{r} \frac{\partial \omega_A}{\partial \theta} \quad (\text{B.3-5})$$

$$j_{Az} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial z} \quad (\text{B.3-6})$$

Spherical coordinates ( $r, \theta, \phi$ ):

$$j_{Ar} = -\rho \mathcal{D}_{AB} \frac{\partial \omega_A}{\partial r} \quad (\text{B.3-7})$$

$$j_{A\theta} = -\rho \mathcal{D}_{AB} \frac{1}{r} \frac{\partial \omega_A}{\partial \theta} \quad (\text{B.3-8})$$

$$j_{A\phi} = -\rho \mathcal{D}_{AB} \frac{1}{r \sin \theta} \frac{\partial \omega_A}{\partial \phi} \quad (\text{B.3-9})$$

<sup>a</sup> To get the molar fluxes with respect to the molar average velocity, replace  $j_A$ ,  $\rho$ , and  $\omega_A$  by  $J_A^*$ ,  $c$ , and  $x_A$ .

§B.4 THE EQUATION OF CONTINUITY<sup>a</sup>

$$[\partial \rho / \partial t + (\nabla \cdot \rho \mathbf{v}) = 0]$$

Cartesian coordinates ( $x, y, z$ ):

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v_x) + \frac{\partial}{\partial y} (\rho v_y) + \frac{\partial}{\partial z} (\rho v_z) = 0 \quad (\text{B.4-1})$$

Cylindrical coordinates ( $r, \theta, z$ ):

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (\rho r v_r) + \frac{1}{r} \frac{\partial}{\partial \theta} (\rho v_\theta) + \frac{\partial}{\partial z} (\rho v_z) = 0 \quad (\text{B.4-2})$$

Spherical coordinates ( $r, \theta, \phi$ ):

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (\rho r^2 v_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\rho v_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} (\rho v_\phi) = 0 \quad (\text{B.4-3})$$

<sup>a</sup> When the fluid is assumed to have constant mass density  $\rho$ , the equation simplifies to  $(\nabla \cdot \mathbf{v}) = 0$ .

§B.5 THE EQUATION OF MOTION IN TERMS OF  $\tau$

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

$$[\rho D\mathbf{v}/Dt = -\nabla p - [\nabla \cdot \boldsymbol{\tau}] + \rho \mathbf{g}]$$

Cartesian coordinates  $(x, y, z)$ :<sup>a</sup>

$$\rho \left( \frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right) = -\frac{\partial p}{\partial x} - \left[ \frac{\partial}{\partial x} \tau_{xx} + \frac{\partial}{\partial y} \tau_{yx} + \frac{\partial}{\partial z} \tau_{zx} \right] + \rho g_x \quad (\text{B.5-1})$$

$$\rho \left( \frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right) = -\frac{\partial p}{\partial y} - \left[ \frac{\partial}{\partial x} \tau_{xy} + \frac{\partial}{\partial y} \tau_{yy} + \frac{\partial}{\partial z} \tau_{zy} \right] + \rho g_y \quad (\text{B.5-2})$$

$$\rho \left( \frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right) = -\frac{\partial p}{\partial z} - \left[ \frac{\partial}{\partial x} \tau_{xz} + \frac{\partial}{\partial y} \tau_{yz} + \frac{\partial}{\partial z} \tau_{zz} \right] + \rho g_z \quad (\text{B.5-3})$$

<sup>a</sup> These equations have been written without making the assumption that  $\boldsymbol{\tau}$  is symmetric. This means, for example, that when the usual assumption is made that the stress tensor is symmetric,  $\tau_{xy}$  and  $\tau_{yx}$  may be interchanged.

Cylindrical coordinates  $(r, \theta, z)$ :<sup>b</sup>

$$\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + v_z \frac{\partial v_r}{\partial z} - \frac{v_\theta^2}{r} \right) = -\frac{\partial p}{\partial r} - \left[ \frac{1}{r} \frac{\partial}{\partial r} (r\tau_{rr}) + \frac{1}{r} \frac{\partial}{\partial \theta} \tau_{\theta r} + \frac{\partial}{\partial z} \tau_{zr} - \frac{\tau_{\theta\theta}}{r} \right] + \rho g_r \quad (\text{B.5-4})$$

$$\rho \left( \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + v_z \frac{\partial v_\theta}{\partial z} + \frac{v_r v_\theta}{r} \right) = -\frac{1}{r} \frac{\partial p}{\partial \theta} - \left[ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{r\theta}) + \frac{1}{r} \frac{\partial}{\partial \theta} \tau_{\theta\theta} + \frac{\partial}{\partial z} \tau_{z\theta} + \frac{\tau_{\theta r} - \tau_{r\theta}}{r} \right] + \rho g_\theta \quad (\text{B.5-5})$$

$$\rho \left( \frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z} \right) = -\frac{\partial p}{\partial z} - \left[ \frac{1}{r} \frac{\partial}{\partial r} (r\tau_{rz}) + \frac{1}{r} \frac{\partial}{\partial \theta} \tau_{\theta z} + \frac{\partial}{\partial z} \tau_{zz} \right] + \rho g_z \quad (\text{B.5-6})$$

<sup>b</sup> These equations have been written without making the assumption that  $\boldsymbol{\tau}$  is symmetric. This means, for example, that when the usual assumption is made that the stress tensor is symmetric,  $\tau_{r\theta} - \tau_{\theta r} = 0$ .

Spherical coordinates  $(r, \theta, \phi)$ :<sup>c</sup>

$$\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_r}{\partial \phi} - \frac{v_\theta^2 + v_\phi^2}{r} \right) = -\frac{\partial p}{\partial r} - \left[ \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \tau_{rr}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\tau_{\theta r} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \tau_{\phi r} - \frac{\tau_{\theta\theta} + \tau_{\phi\phi}}{r} \right] + \rho g_r \quad (\text{B.5-7})$$

$$\rho \left( \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_\theta}{\partial \phi} + \frac{v_r v_\theta - v_\phi^2 \cot \theta}{r} \right) = -\frac{1}{r} \frac{\partial p}{\partial \theta} - \left[ \frac{1}{r^3} \frac{\partial}{\partial r} (r^3 \tau_{r\theta}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\tau_{\theta\theta} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \tau_{\phi\theta} + \frac{(\tau_{\theta r} - \tau_{r\theta}) - \tau_{\phi\phi} \cot \theta}{r} \right] + \rho g_\theta \quad (\text{B.5-8})$$

$$\rho \left( \frac{\partial v_\phi}{\partial t} + v_r \frac{\partial v_\phi}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\phi}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} + \frac{v_\theta v_\phi + v_\theta v_\phi \cot \theta}{r} \right) = -\frac{1}{r \sin \theta} \frac{\partial p}{\partial \phi} - \left[ \frac{1}{r^3} \frac{\partial}{\partial r} (r^3 \tau_{r\phi}) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\tau_{\theta\phi} \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \tau_{\phi\phi} + \frac{(\tau_{\phi r} - \tau_{r\phi}) + \tau_{\phi\theta} \cot \theta}{r} \right] + \rho g_\phi \quad (\text{B.5-9})$$

<sup>c</sup> These equations have been written without making the assumption that  $\boldsymbol{\tau}$  is symmetric. This means, for example, that when the usual assumption is made that the stress tensor is symmetric,  $\tau_{r\theta} - \tau_{\theta r} = 0$ .

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) = -\nabla \cdot \rho \mathbf{v} \mathbf{v} - \nabla p - \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$$

$$\begin{aligned} \frac{\partial}{\partial t} (\rho v_x) &= -\frac{\partial}{\partial x} (\rho v_x v_x) - \frac{\partial}{\partial y} (\rho v_x v_y) - \frac{\partial}{\partial z} (\rho v_x v_z) - \frac{\partial}{\partial x} p - \frac{\partial}{\partial x} \tau_{xx} - \frac{\partial}{\partial y} \tau_{yx} + \rho g_x \quad \text{1-Div} \\ \rightarrow \frac{\partial}{\partial t} (\rho v_x) &= -\frac{\partial}{\partial x} (\rho v_x v_x) - \frac{\partial}{\partial y} (\rho v_x v_y) - \frac{\partial}{\partial z} (\rho v_x v_z) - \frac{\partial}{\partial x} p - \frac{\partial}{\partial x} \tau_{xx} - \frac{\partial}{\partial y} \tau_{yx} \\ &\quad - \frac{\partial}{\partial z} \tau_{zx} + \rho g_x \end{aligned}$$

### §B.6 EQUATION OF MOTION FOR A NEWTONIAN FLUID WITH CONSTANT $\rho$ AND $\mu$

$$[\rho D\mathbf{v}/Dt = -\nabla p + \mu \nabla^2 \mathbf{v} + \rho \mathbf{g}]$$

Cartesian coordinates ( $x, y, z$ ):

$$\rho \left( \frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} \right) = -\frac{\partial p}{\partial x} + \mu \left[ \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right] + \rho g_x \quad (\text{B.6-1})$$

$$\rho \left( \frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} \right) = -\frac{\partial p}{\partial y} + \mu \left[ \frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right] + \rho g_y \quad (\text{B.6-2})$$

$$\rho \left( \frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right) = -\frac{\partial p}{\partial z} + \mu \left[ \frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right] + \rho g_z \quad (\text{B.6-3})$$

Cylindrical coordinates ( $r, \theta, z$ ):

$$\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + v_z \frac{\partial v_r}{\partial z} - \frac{v_\theta^2}{r} \right) = -\frac{\partial p}{\partial r} + \mu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} (r v_r) \right) + \frac{1}{r^2} \frac{\partial^2 v_r}{\partial \theta^2} + \frac{\partial^2 v_r}{\partial z^2} - \frac{2}{r^2} \frac{\partial v_\theta}{\partial \theta} \right] + \rho g_r \quad (\text{B.6-4})$$

$$\rho \left( \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + v_z \frac{\partial v_\theta}{\partial z} + \frac{v_r v_\theta}{r} \right) = -\frac{1}{r} \frac{\partial p}{\partial \theta} + \mu \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} (r v_\theta) \right) + \frac{1}{r^2} \frac{\partial^2 v_\theta}{\partial \theta^2} + \frac{\partial^2 v_\theta}{\partial z^2} + \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} \right] + \rho g_\theta \quad (\text{B.6-5})$$

$$\rho \left( \frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z} \right) = -\frac{\partial p}{\partial z} + \mu \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_z}{\partial \theta^2} + \frac{\partial^2 v_z}{\partial z^2} \right] + \rho g_z \quad (\text{B.6-6})$$

Spherical coordinates ( $r, \theta, \phi$ ):

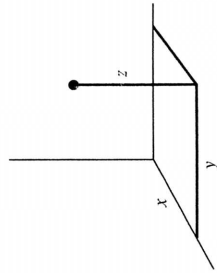
$$\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_r}{\partial \phi} - \frac{v_\theta^2 + v_\phi^2}{r} \right) = -\frac{\partial p}{\partial r} + \mu \left[ \frac{1}{r^2} \frac{\partial^2}{\partial r^2} (r^2 v_r) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial v_r}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 v_r}{\partial \phi^2} \right] + \rho g_r \quad (\text{B.6-7})^a$$

$$\rho \left( \frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_\theta}{\partial \phi} + \frac{v_r v_\theta - v_\phi^2 \cot \theta}{r} \right) = -\frac{1}{r} \frac{\partial p}{\partial \theta} + \mu \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial v_\theta}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left( \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (v_\theta \sin \theta) \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 v_\theta}{\partial \phi^2} + \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} - \frac{2 \cot \theta}{r^2 \sin \theta} \frac{\partial v_\phi}{\partial \phi} \right] + \rho g_\theta \quad (\text{B.6-8})$$

$$\rho \left( \frac{\partial v_\phi}{\partial t} + v_r \frac{\partial v_\phi}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\phi}{\partial \theta} + \frac{v_\phi}{r \sin \theta} \frac{\partial v_\phi}{\partial \phi} + \frac{v_\phi v_r + v_\theta v_\phi \cot \theta}{r} \right) = -\frac{1}{r \sin \theta} \frac{\partial p}{\partial \phi} + \mu \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial v_\phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left( \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (v_\phi \sin \theta) \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 v_\phi}{\partial \phi^2} + \frac{2}{r^2 \sin \theta} \frac{\partial v_r}{\partial \phi} + \frac{2 \cot \theta}{r^2 \sin \theta} \frac{\partial v_\theta}{\partial \phi} \right] + \rho g_\phi \quad (\text{B.6-9})$$

<sup>a</sup> The quantity in the brackets in Eq. B.6-7 is *not* what one would expect from Eq. (M) for  $[\nabla \cdot \nabla \mathbf{v}]$  in Table A.7-3, because we have added to Eq. (M) the expression for  $(2/r)(\nabla \cdot \mathbf{v})$ , which is zero for fluids with constant  $\rho$ . This gives a much simpler equation.

CARTESIAN



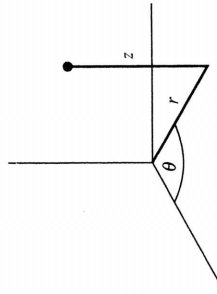
DIVERGENCE

$$\text{div } \mathbf{F} \\ \nabla \cdot \mathbf{F} \quad \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

GRADIENT

$$\text{grad } f \\ \nabla f \quad \begin{aligned} (\text{grad } f)_x &= \frac{\partial f}{\partial x} \\ (\text{grad } f)_y &= \frac{\partial f}{\partial y} \\ (\text{grad } f)_z &= \frac{\partial f}{\partial z} \end{aligned}$$

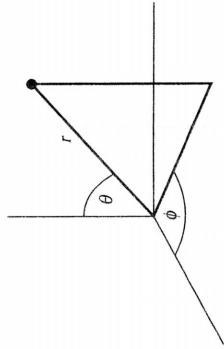
CYLINDRICAL



$$\frac{1}{r} \frac{\partial}{\partial r} (r F_r) + \frac{1}{r} \frac{\partial F_\theta}{\partial \theta} + \frac{\partial F_z}{\partial z}$$

$$\begin{aligned} (\text{grad } f)_r &= \frac{\partial f}{\partial r} \\ (\text{grad } f)_\theta &= \frac{1}{r} \frac{\partial f}{\partial \theta} \\ (\text{grad } f)_z &= \frac{\partial f}{\partial z} \end{aligned}$$

SPHERICAL



$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 F_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta F_\theta) + \frac{1}{r \sin \theta} \frac{\partial F_\phi}{\partial \phi}$$

$$\begin{aligned} (\text{grad } f)_r &= \frac{\partial f}{\partial r} \\ (\text{grad } f)_\theta &= \frac{1}{r} \frac{\partial f}{\partial \theta} \\ (\text{grad } f)_\phi &= \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi} \end{aligned}$$

# Details - Sivab - Zeldovich forms,

- Last lecture we discussed the Derivation of Mass, Species, momentum, energy using the Reynolds Transport Theorem
- These equations are powerful, Physically accurate and provide many levels of Description of Reacting flows - Combustion especially.
- The equations are general for gas-phase. But often more general than we need  $\rightarrow$  simplify them.
- \* An important simplification ~~is~~ is called the Sivab - Zeldovich form of the energy equation.
  - Used in the Description of Premixed and nonpremixed flames to follow.
  - Its not exact, so we Don't use it in computer codes. But the Simplifications make the math easier  $\rightarrow$  Solvable  $\rightarrow$  Theoretical analysis that is very useful for understanding flame behavior.

## Energy Eqn

• 
$$\frac{dpe}{dt} + \nabla \cdot (\rho e \vec{v}) = -\nabla \cdot \vec{q} - \nabla \cdot (\tau \cdot \vec{v}) - \nabla \cdot \vec{p}\vec{v} + \rho \vec{g} \cdot \vec{v}$$

- No shaft work  
 -  $e = h - \frac{p}{\rho} + \frac{1}{2} v^2$   
 -  $\vec{q} = -\lambda \nabla T + \sum h_i \vec{m}_i + \dot{Q}''_{source}$

} General for energy eqn.

• HW  $\rightarrow$  (7.55)

$$\sum \dot{m}_x'' \frac{dh_x}{dx} + \frac{d}{dx} \left( -k \frac{dT}{dx} \right) + \dot{m}_x'' v_x \frac{dv_x}{dx} = - \sum h_x \dot{m}_x''$$

- SS
- No P.E
- 1-D Cartesian
- No  $\dot{Q}''_{source}$
- No viscous Dissipation

• This is a more convenient form.

• HW  $\rightarrow$  (7.67)

$$\dot{m}_x c_p \frac{dT}{dx} + \frac{d}{dx} \left( -\lambda \frac{dT}{dx} \right) + \sum_{i=1}^N \rho Y_i v_i^D c_{p,i} \frac{dT}{dx} = - \sum h_x \dot{m}_x''$$

• look at physical meaning of terms

= 7.55 w/o K.E



Sivash - Zeldovich

- Species mass fluxes, enthalpies eliminated
- enthalpy equation  $\rightarrow$  looks just like the species equation

Start w/ Energy eqn

$\rightarrow$  SS, no KE, PE, Visc Diss,

$$\frac{dpe}{dt} + \nabla \cdot (\rho e \vec{v}) = -\nabla \cdot \vec{q} - \nabla \cdot (\rho \vec{v} \cdot \vec{v}) - \nabla \cdot (\rho \vec{v} \cdot \vec{v}) + \rho \vec{v} \cdot \vec{v}$$

$$\nabla \cdot (\rho v h) - \nabla \cdot (\rho v) \quad \text{w/o KE}$$

$$\boxed{\nabla \cdot (\rho v h) = -\nabla \cdot \vec{q}}$$

Turns 7.51

Convection + Diffusion = 0

Heat Flux

$$\boxed{\vec{q} = -\lambda \nabla T + \sum j_i h_i}$$

- Assume  $j_i = -\rho D_i \nabla Y_i$
- Assume all  $D_i$ 's are equal  $\rightarrow D$
- Assume Unity  $Le$ ;  $Le = 1 = \frac{\alpha}{D} = \frac{\lambda}{\rho C_p D} = 1 \rightarrow \alpha = D$

$$\vec{q} = -\lambda \nabla T - \sum \rho D (h_i \nabla Y_i)$$

Now:  $\nabla Y_i h_i = (h_i \nabla Y_i) + Y_i \nabla h_i \rightarrow (h_i \nabla Y_i) = \nabla Y_i h_i - Y_i \nabla h_i$

$$\vec{q} = -\lambda \nabla T - \sum \rho D \overset{①}{\nabla Y_i h_i} + \sum \rho D \overset{②}{Y_i \nabla h_i}$$

①: • Pull  $\sum$  inside  $\nabla$  (This works cause  $D_i = D$  (all same))

$$\rightarrow \nabla \sum Y_i h_i = \nabla h$$

②: • Also  $\nabla h_i = C_{p,i} \nabla T \rightarrow \rho D \sum Y_i C_{p,i} \nabla T \rightarrow \rho D C_p \nabla T$

$$\vec{q} = -\lambda \nabla T - \rho D \nabla h + \rho D C_p \nabla T$$

• but  $\rho D C_p = \lambda$  by  $Le = 1$

$$\boxed{\vec{q} = -\rho D \nabla h}$$

nice!

Insert :

$$\boxed{\nabla \cdot (\rho \vec{V} h) = \nabla \cdot \rho D \nabla h} \quad \equiv \text{Turns } 7.81, 7.82, 7.83$$

or

$$\rho \vec{V} \cdot \nabla h = \nabla \cdot \rho D \nabla h$$

• Note  $\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{V} = 0$  Continuity Mass  
 $\rightarrow \rho \vec{V}$  is constant

- Enthalpy is a Conserved Scalar under our assumptions
- e.g.  $\nabla \cdot (\rho \vec{V} h) - \nabla \cdot \rho D \nabla h = 0$  ;  $h$  is only transported
  - There are no Sources and no Sinks.
  - Its transported as a whole, not as a collection of species enthalpies that all go "out of sync." This is due to the  $Le = 1$  assumption for all species.

• Now write in terms of  $h_{sensible}$  :  $h = h_f + h_{sens}$

$\rightarrow$  replace the  $h$  w/  $h_s$ , but get a source term to account for conversion of internal and sensible.

$\rightarrow$  Shvab - Zeldovich.

$$\rho \vec{V} \cdot \nabla h_s + \boxed{\rho \vec{V} \cdot \nabla h_f} = \nabla \cdot \rho D \nabla h_s + \boxed{\nabla \cdot \rho D \nabla h_f}$$

$h_f = \sum Y_k h_{f,k}^o$  but  $h_{f,k}^o$  is constant  $\rightarrow$  pull out of  $\nabla$

$$\begin{aligned} \rho \vec{V} \cdot \nabla h_s - \nabla \cdot \rho D \nabla h_s &= -(\rho \vec{V} \cdot \nabla h_f - \nabla \cdot \rho D \nabla h_f) \\ &= -\left( \sum (\rho \vec{V} h_{f,k} \nabla Y_k - h_{f,k} \nabla \cdot \rho D \nabla Y_k) \right) \\ &= -\sum h_{f,k} (\rho \vec{V} \nabla Y_k - \nabla \cdot \rho D \nabla Y_k) \\ &= -\sum h_{f,k} \underbrace{\dot{m}_k'''}_{\dot{m}_k'''} \end{aligned}$$

$$\boxed{\rho \vec{V} \cdot \nabla h_s - \nabla \cdot \rho D \nabla h_s = -\sum h_{f,k}^o \dot{m}_k'''} \quad \equiv \text{Shvab - Zeldovich Energy Eq.}$$

•  $h_s = \int_{T_{ref}}^T C_p dT$

Turns (7.64) (7.65) (7.66) (7.63)

Note:  $h_s = \int_{T_{ref}}^T c_p dT \rightarrow \frac{dh_s}{dx} = \frac{d}{dx} \int_{T_{ref}}^T c_p dT = c_p \frac{dT}{dx}$

$\nabla h_s \rightarrow c_p \nabla T$

$\rho \vec{V} \cdot \nabla h_s - \nabla \cdot \rho D c_p \nabla T = - \sum h_{f,i} \dot{m}_i'''$

- used in Planmixed flames Turns (8.7a)

Compare energy and species.

$h: \rho \vec{V} \cdot \nabla h_s - \nabla \cdot \rho D \nabla h_s = - \sum h_{f,i} \dot{m}_i'''$

$Y_x: \rho \vec{V} \cdot \nabla Y_x - \nabla \cdot \rho D \nabla Y_x = \dot{m}_x'''$

(Convection) (Diffusion) (Source)

Note Signs

- Creation of internal energy =  
+ Creation of sensible

Axisymmetric:



$\nabla f \rightarrow \frac{\partial f}{\partial x} + \frac{\partial f}{\partial r}$

$\nabla \cdot \vec{f} \rightarrow \frac{1}{r} \frac{\partial}{\partial r} (r f_r) + \frac{\partial}{\partial x} f_x$

$\frac{1}{r} \frac{\partial}{\partial r} (r \rho V_r h_s) + \frac{\partial}{\partial x} (\rho V_x h_s) - \nabla \cdot \left( \rho D \frac{\partial h_s}{\partial x} + \rho D \frac{\partial h_s}{\partial r} \right) = - \sum h_{f,i} \dot{m}_i'''$

$= \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho D \frac{\partial h_s}{\partial x} + r \rho D \frac{\partial h_s}{\partial r} \right)$

$= \frac{\partial}{\partial x} \left( \rho D \frac{\partial h_s}{\partial x} + \rho D \frac{\partial h_s}{\partial r} \right)$

$\frac{1}{r} \frac{\partial}{\partial r} (r \rho V_r h_s) + \frac{\partial}{\partial x} (\rho V_x h_s) - \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho D \frac{\partial h_s}{\partial x} + r \rho D \frac{\partial h_s}{\partial r} \right) - \frac{\partial}{\partial x} \left( \rho D \frac{\partial h_s}{\partial x} + \rho D \frac{\partial h_s}{\partial r} \right) = - \sum h_{f,i} \dot{m}_i'''$

Turns only keeps this term.

- Boundary-Layer approximation.