Energy Eq — Recap @ Class 21

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

S.S. ; no K.E. ; no Dissipation by μ ; no P.E.

$$\nabla\cdot(\rho e\vec{v}) = -\nabla\cdot q - \nabla\cdot p\vec{v}$$

$$e = u = h - \frac{p}{\rho}$$

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

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

$$q = -\lambda\nabla T + \sum j_i h_i$$

for $j_i = -\rho D_i \nabla Y_i$, $D_i = \frac{\lambda}{\rho c_p}$ ($Le_i = 1$)

$$q = -\rho D \nabla h$$

$$\boxed{\nabla\cdot(\rho\vec{v}h) - \nabla\cdot(\rho D\nabla h) = 0}$$

for h_{sens}:

$$\rho\vec{v}\cdot\nabla h_s - \nabla\cdot(\rho D\nabla h_s) = -\sum h^{o}_{fi}\, \dot{m}_i'''$$ → Shvab-Zeld.

Compare Species

$$\rho\vec{v}\cdot\nabla Y_i - \nabla\cdot(\rho D\nabla Y_i) = \dot{m}_i'''$$

· Very similar. (note sign)

Note $\nabla h_s = c_p \nabla T$ since $h_s = \int_{T_r}^{T} c_p\, dT$

These similarities → same soln form of PDE's for flames.

Lecture 21

Conserved Scalar

Last time we Derived the following Transport equation for enthalpy

$$\nabla\cdot(\rho v h) - \nabla\cdot\rho D\nabla h = 0$$

- ss
- no KE, PE, visc, W_s, Radiation
- $Le_i = 1$

Q: What indicates a Conserved Scalar here?
- Only Transport, no Sources, no Sinks.
- Key enabler is $Le_i = 1$
- Also, can have an unsteady version of this.

- Other Conserved Scalars?
  - Elemental mass fractions
  - ↓
  - Mixture fraction.

- Conserved Scalars can significantly Simplify analysis of Combustion Systems, - especially nonpremixed flames

  * - We have seen how we can represent h, T, Y_i as functions of ξ via assumptions like equilibrium. Then, if we knew ξ everywhere (via its Transport equation) we could get $\phi(\xi)$ everywhere.
  - This is routinely Done in Turbulent non-premixed flames.

ξ - Transport equation

Species Transport Eqn:

$$(1)\quad \frac{\partial \rho Y_i}{\partial t} + \nabla\cdot(\rho Y_i v) - \nabla\cdot(\rho D\nabla Y_i) = \dot{m}_i'''$$

Assumes
$j = -\rho D_i \nabla Y_i$
$D_i \equiv D$ (uniform D)

$$\xi = \frac{Z_k - Z_k^o}{Z_k^1 - Z_k^o} \quad ; \quad Z_k = \sum_{i=1}^{N_{sp}} a_{k,i}\frac{M_k}{M_i}Y_i$$

- $a_{k,i}$, M_k, M_i, Z_k^o, $(Z_k^1 - Z_k^o)$ are <u>all</u> constants.

- Multiply (1) by $a_{k,i} \frac{M_k}{M_i}$
- Sum over all i
- Pull the Sum inside Derivatives.
- $\sum a_{ki} \frac{M_k}{M_i} \dot{m}_i''' = \dot{m}_k''' = 0$; Elements Don't react!

$$* \quad \frac{\partial \rho Z_k}{\partial t} + \nabla \cdot (\rho Z_k v) - \nabla \cdot (\rho D \nabla Z_k) = 0$$

- Subtract Z_k^0 (its constant → pull inside Derivatives)
- $\div$ $Z_k^1 - Z_k^0$ (again Const. → ")

$$\boxed{\frac{\partial \rho \xi}{\partial t} + \nabla \cdot (\rho v \xi) - \nabla \cdot (\rho D \nabla \xi) = 0}$$

= Turns (7.77)
(7.78)
(7.79)

- Assumes $J = -\rho D_i \nabla Y_i$
- Assumes uniform D_i → $D_i = D$

otherwise we can't pull $\sum_i$ inside second ∇ in the Diffusive Term.

→ ξ is a conserved scalar.

Elements rearrange among species via Rxn, but elements stay in ratio dictated by pure mixing.

The Elements "Diffuse in Sync" so to speak.

- What to use for D? usually use α → $\frac{\alpha}{D} = Le = 1$
- * If know any (1) Conserved Scalar, know all the others.

$\xi \to Z_k$ under given assumptions.

$\to h$

Laminar flamelet equations

- Flames are usually thin → 1-D $\perp$ to flame sheet.
- 1-D species eqn:

$$\frac{\partial \rho Y_i}{\partial t} + \frac{\partial}{\partial x}(\rho Y_i v) - \frac{\partial}{\partial x}\left(\rho D \frac{\partial}{\partial x} Y_i\right) = \dot{m}_i'''$$

Note: we said we can transport ξ, and if $Y_i = Y_i(\xi)$ then we can simplify combustion by transporting only ξ, and get Y_i as $Y_i(\xi)$.

* Convert the above eqn for $Y_i(t,x)$ to $Y_i(t,\xi)$

Consider the S.S. version → $Y_i(x) \to Y_i(\xi)$

$$\xi = \xi(x) \to d\xi = \frac{\partial \xi}{\partial x} dx \to \frac{d}{dx} = \frac{d\xi}{dx}\frac{d}{d\xi}$$

$$\to \frac{d\xi}{d\phi} = \frac{\partial \xi}{\partial x}\frac{dx}{d\phi} \to \frac{d\phi}{dx} = \frac{d\xi}{dx}\frac{d\phi}{d\xi}$$

Apply this:

$$\frac{d\xi}{dx}\frac{d}{d\xi}(\rho Y_i v) - \underbrace{\frac{d\xi}{dx}\frac{d}{d\xi}\left(\rho D \frac{d\xi}{dx}\frac{d}{d\xi} Y_i\right)} = \dot{m}_i'''$$

$$\rho v \frac{\partial Y_i}{\partial x} \to \rho v \frac{\partial \xi}{\partial x}\frac{\partial Y_i}{\partial \xi} \to \frac{\partial \rho v \xi}{\partial x}\frac{\partial Y_i}{\partial \xi}$$

$$\underbrace{\frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi}(\rho v Y_i)} - \frac{\partial \xi}{\partial x}\frac{\partial Y_i}{\partial \xi}\frac{\partial}{\partial \xi}\left(\rho D \frac{\partial \xi}{\partial x}\right) - \rho D\left(\frac{\partial \xi}{\partial x}\right)^2 \frac{\partial^2 Y_i}{\partial \xi^2} = \dot{m}_i'''$$

$$\underbrace{\frac{\partial Y_i}{\partial \xi}\left(\frac{\partial \rho v \xi}{\partial x} - \underbrace{\frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi}}_{\frac{\partial}{\partial x}}\left(\rho D \frac{\partial \xi}{\partial x}\right)\right)}_{=0 \text{ via } \xi \text{ transport equation}} - \rho D\left(\frac{\partial \xi}{\partial x}\right)^2 \frac{\partial^2 Y_i}{\partial \xi^2} = \dot{m}_i'''$$

$$\to \boxed{\rho D\left(\frac{\partial \xi}{\partial x}\right)^2 \frac{\partial^2 Y_i}{\partial \xi^2} = -\dot{m}_i'''}$$

- Unsteady version too. →

$$\underbrace{D\left(\frac{\partial \xi}{\partial x}\right)^2} \frac{\partial^2 Y_1}{\partial \xi^2} = \frac{-\dot{m}_1'''}{\rho}$$

Let $\chi = 2D\left(\frac{\partial \xi}{\partial x}\right)^2$

$$\rightarrow \boxed{\frac{\chi}{2} \frac{\partial^2 Y_1}{\partial \xi^2} = -\frac{\dot{m}_1'''}{\rho}}$$

- χ is Scalar Dissipation Rate
- $\chi \left(=\right) \frac{1}{s}$
- χ is a mixing timescale.
- Looks like $\frac{1}{\tau}$ in PSR eqns
- χ is Treated as a parameter.

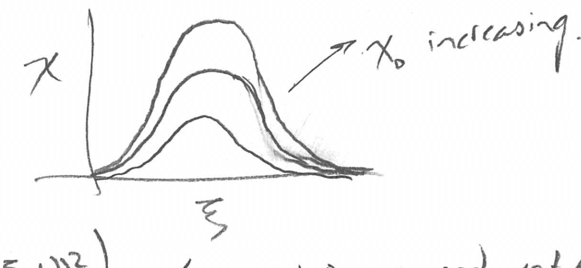
Solve These eqns for each χ.

1-D in ξ,

$\rightarrow Y_1 = Y_1(\xi, \chi)$

(Actually $\chi = \chi(\xi) = \chi_0 f(\xi)$ where $\chi_0 =$ Constant $\rightarrow$

$Y_1 = Y_1(\xi, \chi_0)$



$\chi = \chi_0 \exp\left(-2\left(\mathrm{erf}^{-1}(2\xi - 1)\right)^2\right)$ for 1-D opposed jet flames.

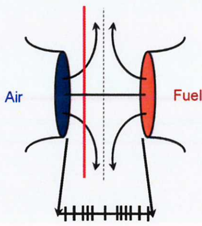
. if assume $\xi(x)$ is a tanh function instead of an error function

$\chi = \chi_0\left(1 - (2\xi - 1)^2\right)^2$

$\boxed{\text{See PPT}}$

Flamelet Modeling

- Flamelets transform physical coordinate to flame coordinate.
- Assumes unity Le



$$\rho\frac{\partial Y_i}{\partial t} = \rho v\frac{\partial Y_i}{\partial y} + \frac{\partial}{\partial y}\left(\rho D\frac{\partial Y_i}{\partial y}\right) + \omega_i$$

$$\chi = 2D\left(\frac{\partial \xi}{\partial y}\right)^2$$

$$\frac{\partial Y_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 Y_i}{\partial \xi^2} + \omega_i/\rho$$

Define mixture fraction f by transport equation

$$* \quad \rho\frac{\partial \xi}{\partial t} + \rho v\frac{\partial \xi}{\partial y} - \frac{\partial}{\partial y}\left(\rho D_\xi\frac{\partial \xi}{\partial y}\right) = 0$$

Species transport equation

$$\rho\frac{\partial Y_i}{\partial t} = \rho v\frac{\partial Y_i}{\partial y} + \frac{\partial}{\partial y}\left(\rho D\frac{\partial Y_i}{\partial y}\right) + \omega_i$$

Coordinate transformation

$$\frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial t} + \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi} \qquad \frac{\partial}{\partial y} \rightarrow \frac{\partial \xi}{\partial y}\frac{\partial}{\partial \xi}$$

Apply (*) and rearrange

$$\frac{\partial Y_i}{\partial t} = \frac{\chi}{2}\frac{\partial^2 Y_i}{\partial \xi^2} + \omega_i/\rho \qquad \chi = 2D\left(\frac{\partial \xi}{\partial y}\right)^2$$