<Conservation Equations>

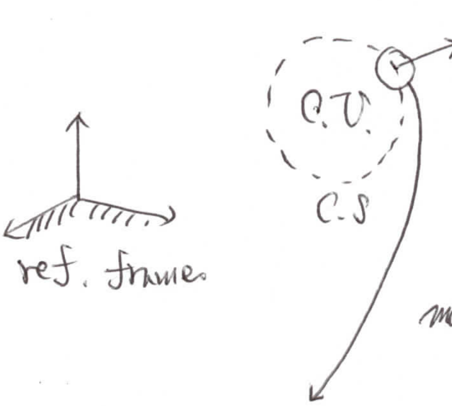
* for reacting ideal gas mixture.

Let's develop mathematical forms of the conservation eqns. needed to describe the combined influence of chemistry, mass/heat transfer on combustion phenomena.

- total mass, momentum and energy of a reacting flow are conserved
- species mass fractions are related by stoichiometries of the chemical rxns and the species-specific transport rates.

  ⇒ production/destruction + transport.

◎ General forms of the conservation Eqns.



$\vec{v}_i$

species velocity of species i

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

$\vec{v}$: mass-averaged velocity

$\vec{V}_i$: Diffusion velocity.

dA

$\vec{n}$: normal unit vector ($|\vec{n}| = 1$)

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

⇒ flux $= X \cdot (\vec{v} + \vec{V}_i) \cdot \vec{n} \times dA$ (X: a property)

* We need to consider production from chemical reactions.

flux (X) + rate of accumulation (X) = rate of production (X)

X can be total mass, species mass, momentum or energy

- Conservation of mass.

  rate of production $=0$.

$$\underset{C.S.}{\iint} \sum_i \rho_i (\vec{v} + \vec{V_i}) \cdot \vec{n}\, dA + \frac{\partial}{\partial t} \underset{CV}{\iiint} \sum_i \rho_i \, dV = 0$$

C.S. control surface; $\cdot$ dot product; $\frac{\partial}{\partial t}$ rate; dV volume.

$$\sum_i \rho_i = \rho, \quad \sum_i \rho_i \vec{V_i} = \underbrace{\sum_i J_i''}_{\text{see previous handout.}} = 0$$

$\rightarrow$ No net mass transport by molecular diffusion.

$$\therefore \underbrace{\underset{C.S.}{\iint} \rho \vec{v} \cdot \vec{n}\, dA}_{} + \underset{CV}{\iiint} \underbrace{\left(\frac{\partial \rho}{\partial t}\right) dV}_{} = 0.$$

$\because V$ is not a function of t. (Control volume)

Divergence theorem ($\iint \vec{B} \cdot \vec{n}\, dA = \iiint (\nabla \cdot \vec{B})\, dV$.)

$\rightarrow \iiint \nabla \cdot (\rho \vec{v})\, dV$

$$\therefore \underline{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0}$$

if steady state $\Rightarrow \frac{\partial \rho}{\partial t} = 0$

$\therefore \underline{\nabla \cdot (\rho \vec{v}) = 0.}$ //

- Conservation of momentum.

* rate of momentum production $= \frac{\partial (mv)}{\partial t} = \underline{\text{force}}$ //

$=$ body force (e.g., gravity), viscous force, pressure (normal or shear)

$X_i = \rho_i \vec{V_i}$, $\sum_i$ (eqn) $\Rightarrow$ <u>Navier-Stokes eqn.</u> //

$$\rho \frac{\partial \vec{v}}{\partial t} + \rho \vec{v} \cdot \nabla \vec{v} = -\nabla \cdot \vec{P} + \underbrace{\rho \sum_i Y_i f_i}_{\text{Body force}}$$

$\vec{P}$: stress tensor.

for a steady, inviscid flow without body force.

$$\underline{\nabla p + \rho \vec{v}\cdot\nabla\vec{v} = 0}$$

Euler's equation.

- Conservation of species

* chemical reaction serves as a source/sink of a species i

= rate of production of species i per volume

$= \hat{RR}_i''' \hat{M}_i$ = mass production

$\rho \cdot Y_i$ = mass fraction; $\hat{RR}_i'''$ ↑ mole; $\hat{M}_i$ ↑ molar mass of i

$$\frac{\partial \rho_i}{\partial t} + \nabla\cdot(\rho_i(\vec{v}+\vec{V}_i)) \leftarrow \underline{\frac{\partial \rho_i}{\partial t} + \nabla\cdot(\rho_i \vec{v}_i) = \hat{RR}_i''' \cdot \hat{M}_i}$$

↑ We learned how to estimate rxn rate.

- Conservation of energy.

$$e_i = \underbrace{u_{i,\text{sensible}} + e_{i\,\text{chem.}}}_{\text{conversion between these two are already considered}} + \underbrace{\tfrac{1}{2}V^2}_{\text{kinetic energy}}, \quad \sum_i \rho_i e_i = \rho e$$

$$\underbrace{\frac{\partial(\rho e)}{\partial t}}_{\text{rate of energy accumulation}} + \underbrace{\nabla\cdot\left(\sum_i \rho_i \vec{v}_i e_i\right)}_{\text{energy transport by bulk flow and diffusion}} + \underbrace{\nabla\cdot\left(\sum_i P_i \vec{v}_i\right)}_{\text{work rate by pressure force}} + \underbrace{\nabla\cdot\vec{q}}_{\text{heat flux}} = 0$$

$$\vec{v}_i = \vec{v} + \vec{V}_i, \quad h = u + P/\rho, \quad \tfrac{1}{2}V^2 \approx 0.$$

$$\Rightarrow \underline{\underbrace{\frac{\partial(\rho h)}{\partial t} - \frac{\partial P}{\partial t}}_{\text{unsteady terms}} + \nabla\cdot\left(\rho\vec{v}h + \sum_i \rho_i \vec{V}_i h_i\right) + \nabla\cdot\vec{q} = 0}$$

◎ Shvab – Zeldovich Formulation.

* $\vec{V_i}$ and $\vec{q}$ should be expressed for further proceeding.

⇒ assume Fickian mass diffusion and Fourier heat conduction.

$$\vec{J_i}'' = \rho_i \vec{V_i} = -\rho D_{ij} \nabla Y_i$$

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

⇒ Assume steady state

∘ Species conservation + Energy conservation

$$\nabla \cdot (\underbrace{\rho \vec{v} Y_i}_{=\rho_i \vec{v}} - \rho D_{ij} \vec{\nabla} Y_i) = \vec{RR_i}''' \hat{M_i}$$

$$\nabla \cdot (\rho \vec{v} h - \rho \sum_i h_i D_{ij} \nabla Y_i - \lambda \nabla T) = 0$$

$\Delta_f H_i$ (formation energy of species i per unit mass)

$$h = \sum_i Y_i h_i = \sum_i Y_i (h_{i,sens} + \Delta_f H_i(T_{ref}))$$

$$= \underline{h_{sens} + \sum_i Y_i \Delta_f H_i(T_{ref})}$$

$\vec{RR_i}''' = (\nu_i' - \nu_i) RR'''$

assume. $D_{ij} = D$ = average binary diffusion coefficient.

assume ideal gas ⇒ $h_{i,sens} \underset{\uparrow}{=} h_i(T)$ ∴ $\nabla h_{i,sens} = C_{p_i}(T) \nabla T$

only the function of T

Define $\eta_i \equiv \dfrac{Y_i}{(\nu_i' - \nu_i)\hat{M_i}}$, $\eta_T \equiv \dfrac{h_{sens}}{-\Delta H_R}$

⇒ $\boxed{\begin{array}{l} \text{Cons. of species} : \nabla \cdot (\rho \vec{v} \eta_i - \rho D \nabla \eta_i) = RR''' \\ \text{Cons. of energy} : \nabla \cdot (\rho \vec{v} \eta_T - \rho D \nabla \eta_T) = RR''' \end{array}}$

$$\therefore L(\eta) = RR'''$$