Transport Equations

1 Mass Conservation

Details could be found in **Viscous Flow Continuity** section. In this chapter, we use v to replace u. Recall:

$$\overbrace{0}^{production} = \overbrace{\frac{\partial \rho}{\partial t}}^{change} + \overbrace{\nabla \cdot (\rho \underline{\boldsymbol{v}})}^{flux(out)} \tag{1}$$

2 Velocity

In combustion process, total velocity should be "sum" of all species in mixture.

Mass Average Velocity:

$$\underline{\boldsymbol{v}} = \frac{\sum \rho_i \underline{\boldsymbol{v_i}}}{\sum \rho_i} = \frac{\sum \rho_i \underline{\boldsymbol{v_i}}}{\rho} = \sum Y_i \underline{\boldsymbol{v_i}} \tag{2}$$

Mass Diffusion Velocity:

$$\underline{\boldsymbol{V_i}} = \underline{\boldsymbol{v_i}} - \underline{\boldsymbol{v}} \tag{3}$$

Mole Average Velocity:

$$\underline{\boldsymbol{v}^*} = \sum X_i \underline{\boldsymbol{v_i}} \tag{4}$$

Molar Diffusion Velocity:

$$\underline{\boldsymbol{V_i^*}} = \underline{\boldsymbol{v_i}} - \underline{\boldsymbol{v}^*} \tag{5}$$

3 Species Conservation

Species conservation could be derived from mass conservation. For each species:

$$\overbrace{\dot{m}_i'''}^{production} = \overbrace{\frac{\partial \rho_i}{\partial t}}^{change} + \overbrace{\nabla \cdot (\rho_i \underline{\boldsymbol{v_i}})}^{flux(out)} \tag{6}$$

Here $\dot{m}_i'''$ is the source term, with the unit as $kg/(m^3 \cdot s)$. It can also be expressed as:

$$\dot{m}_i''' = \bar{W}_i \dot{\omega}_i \tag{7}$$

Here:

1. $\bar{W}_i$ is the molar mass of the species, with unit as $kg/mole$.
2. $\dot{\omega}_i$ is the rate of change of the concentration, with the unit as $mole/(m^3 \cdot sec)$

$$\dot{\omega}_i = \frac{d[M_i]}{dt} = (v''_{ji} - v'_{ji})\{k_{jf} \prod [M_i]^{v'_{ji}} - k_{jr} \prod [M_i]^{v''_{ji}}\} \tag{8}$$

$$\frac{dY_i}{dt} = \dot{\omega}_i \frac{\bar{W}_i}{\rho} \tag{9}$$

Then, from the previous section, the species velocity is:

$$\underline{\boldsymbol{v_i}} = \underline{\boldsymbol{V_i}} + \underline{\boldsymbol{v}} \tag{10}$$

Plug back in:

$$\begin{aligned}\bar{W}_i \dot{\omega}_i &= \frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i (\underline{\boldsymbol{V_i}} + \underline{\boldsymbol{v}})) \\ &= \rho \frac{\partial Y_i}{\partial t} + \rho \underline{\boldsymbol{v}} \cdot \nabla Y_i + \nabla \cdot (\rho Y_i \underline{\boldsymbol{V_i}}) + \cancelto{0}{Y_i \frac{\partial \rho}{\partial t} + Y_i \nabla \cdot (\rho \underline{\boldsymbol{v}})}\end{aligned} \tag{11}$$

Therefore:

$$\bar{W}_i \dot{\omega}_i = \underbrace{\rho \frac{DY_i}{Dt}}_{\text{change+conv flux}} + \underbrace{\nabla \cdot (\rho Y_i \underline{\boldsymbol{V_i}})}_{\text{diffusive flux}} \tag{12}$$

4 Diffusive Fluxes

Diffusive Mass Flux:

$$\underline{\boldsymbol{j_i}} = \rho Y_i \underline{\boldsymbol{V_i}} = \rho Y_i (\underline{\boldsymbol{v_i}} - \underline{\boldsymbol{v}}) \tag{13}$$

Here $\underline{\boldsymbol{j_i}}$ has the unit as $kg/(m^2 \cdot s)$, meets the definition of mass flux.
Diffusive Molar Flux:

$$\underline{\boldsymbol{J_i^*}} = [M] X_i \underline{\boldsymbol{V_i^*}} = [M] X_i (\underline{\boldsymbol{v_i}} - \underline{\boldsymbol{v^*}}) \tag{14}$$

Here:

1. $\underline{\boldsymbol{J_i^*}}$ has the unit as $mole/(m^2 \cdot s)$, meets the definition of molar flux.
2. X_i is the molar fraction, dimensionless.
3. $[M]$ is the concentration, with the unit as $mole/m^3$

In average reference frame, sum of all diffusive fluxes leads to no net transport of total mass (or moles), so:

$$\sum \underline{\boldsymbol{J_i^*}} = \sum \underline{\boldsymbol{j_i}} = 0 \tag{15}$$

For the simple binary systems, recall the Fick's Law:

$$\underline{\boldsymbol{j_i}} = -\rho D_{ij} \nabla Y_i \tag{16}$$

Where D_{ij} is the binary diffusivity of species i in otherwise pure j. Therefore:

$$\underline{\boldsymbol{j_i}} = -\rho D_{ij} \nabla Y_i = \rho Y_i \underline{\boldsymbol{V_i}} \tag{17}$$

Therefore, we can get the mass diffusion velocity:

$$\underline{\boldsymbol{V_i}} = -D_{ij} \frac{\nabla Y_i}{Y_i} = -D_{ij} \nabla ln Y_i \tag{18}$$

Similarly, we can get the molar diffusion velocity:

$$\underline{\boldsymbol{V_i^*}} = -D_{ij} \nabla ln X_i \tag{19}$$

5 Momentum Conservation

Details in Viscous Flow NS Equations chapter. For species:

$$\rho \sum_i Y_i \underline{\boldsymbol{f_i}} = \rho \frac{D\underline{\boldsymbol{v}}}{Dt} + \nabla \cdot \underline{\underline{\boldsymbol{\tau}}} \tag{20}$$

6 Energy Conservation

Details in Viscous Flow Energy chapter. With the following assumptions (Neglect):

1. Kinetic energy and potential energy
2. Radiation
3. Viscous dissipation and any work but flow work
4. Dufour effect

We can get the simplified energy equation:

$$\rho \frac{Dh}{Dt} = \frac{Dp}{Dt} + \nabla \cdot (k \nabla T) - \sum \nabla \cdot h_i \underline{\boldsymbol{j_i}} \tag{21}$$

7 Unity Lewis Approximation

Enthalpy of mixture:

$$dh = c_p dT + \sum_i h_i dY_i \tag{22}$$

Therefore:

$$\begin{aligned} k\nabla T - \sum h_i \underline{\boldsymbol{j_i}} &= k(\frac{\nabla h}{c_p} - \sum \frac{h_i}{c_p}\nabla Y_i) - \sum h_i \underline{\boldsymbol{j_i}} \\ &= \frac{k}{c_p}\nabla h - \sum h_i(\underline{\boldsymbol{j_i}} + \frac{k}{c_p}\nabla Y_i) \end{aligned} \tag{23}$$

Recall the definition of Lewis number:

$$Le = \frac{\alpha}{D} = \frac{k}{\rho c_p D} \tag{24}$$

and:

$$\underline{\boldsymbol{j_i}} = -\rho D_{ij}\nabla Y_i = -\frac{k}{c_p Le}\nabla Y_i \tag{25}$$

Therefore:

$$\sum h_i(\underline{\boldsymbol{j_i}} + \frac{k}{c_p}\nabla Y_i) = \sum h_i \frac{k}{c_p}(1 - \frac{1}{Le})\nabla Y_i \tag{26}$$

If we assume $Le = 1$, **we mean all species have same mass diffusivity, and no net flux due to chem/c_p difference**, and the above equation will be zero. The energy conservation equation now is:

$$\frac{Dh}{Dt} = \frac{1}{\rho}\frac{Dp}{Dt} + \nabla \cdot (\alpha \nabla h) \tag{27}$$

8 Temperature Equation

Also start from equation:

$$dh = c_p dT + \sum_i h_i dY_i \tag{28}$$

Transfer this to material derivative:

$$\frac{Dh}{Dt} = c_p \frac{DT}{Dt} + \sum_i h_i \frac{DY_i}{Dt} \tag{29}$$

Recall the species conservation equation:

$$\bar{W}_i\dot{\omega}_i = \underbrace{\rho\frac{DY_i}{Dt}}_{\text{change+conv flux}} + \underbrace{\nabla\cdot(\rho Y_i \underline{\boldsymbol{V_i}})}_{\text{diffusive flux}} \tag{30}$$

$$\frac{DY_i}{Dt} = \frac{1}{\rho}(\bar{W}_i\dot{\omega}_i - \nabla\cdot(\rho Y_i \underline{\boldsymbol{V_i}})) \tag{31}$$

Also, we know the mass diffusive flux is:

$$\underline{\boldsymbol{j_i}} = \rho Y_i \underline{\boldsymbol{V_i}} \tag{32}$$

Therefore:

$$\frac{Dh}{Dt} = c_p\frac{DT}{Dt} + \frac{1}{\rho}\sum(\bar{W}_i\dot{\omega}_i - \nabla\cdot\underline{\boldsymbol{j_i}}) \tag{33}$$

Plug it into energy equation, we can get the temperature equation:

$$\rho c_p\frac{DT}{Dt} = \frac{Dp}{Dt} + \nabla\cdot(k\nabla T) - \sum c_{p_i}\underline{\boldsymbol{j_i}}\cdot\nabla T - \sum \bar{W}_i\dot{\omega}_i h_i \tag{34}$$

Here:

1. $\frac{Dp}{Dt}$: compressive work
2. $\nabla\cdot(k\nabla T)$: thermal conduction
3. $\sum c_{p_i}\underline{\boldsymbol{j_i}}\cdot\nabla T$: diffusion of sensible enthalpy by mass
4. $\sum \bar{W}_i\dot{\omega}_i h_i$: chemical energy conversion

If we assume small pressure change and small c_p variations:

$$c_{p_i} \approx c_p \tag{35}$$

Also we know the total mass diffusive fluxes should be zero:

$$\sum \underline{\boldsymbol{j_i}} = 0 \tag{36}$$

Therefore:

$$\begin{aligned}\rho\frac{DT}{Dt} &= \frac{1}{c_p}\nabla\cdot(k\nabla T) - \sum\frac{c_{p_i}}{c_p}\underline{\boldsymbol{j_i}}\cdot\nabla T - \sum\bar{W}_i\dot{\omega}_i\frac{h_i}{c_p} \\ &\approx \nabla\cdot(\frac{k}{c_p}\nabla T) - \sum\bar{W}_i\dot{\omega}_i\frac{h_i}{c_p}\end{aligned} \tag{37}$$

9 Shvab-Zeldovich Formulation

If we assume:

1. Steady flow
2. No body forces
3. Normal diffusion
4. Ignore radiation and viscous dissipation
5. 1D to describe all mas diffusion

We can get the simplified energy equation:

$$\nabla \cdot (\rho \underline{\boldsymbol{v}} h_{sens} - \rho\alpha\nabla h_{sens}) = -\sum h^o_{i,f}\bar{W}_i\dot{\omega}_i \tag{38}$$

and species equation:

$$\nabla \cdot (\rho \underline{\boldsymbol{v}} Y_i - \rho D\nabla Y_i) = \bar{W}_i\dot{\omega}_i \tag{39}$$

If we assume unity Lewis number, $\alpha = D$, these two equations are similar.
Approximate values for various species in CH4-air flame:

	Le_i		Le_i
CO_2	1.39	HCO	1.27
O_2	1.11	CO	1.10
H_2O	0.83	OH	0.73
CH_4	0.97	O	0.70
H_2	0.30	H	0.18

Therefore, we can see that unity Lewis number assumption okay except for light species.