Assignment III

Combustion, Explosion and Detonation

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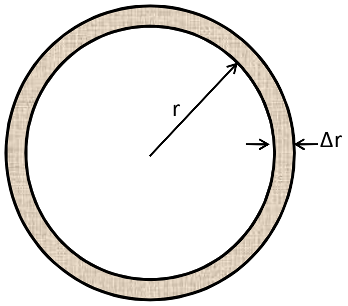
1. **Solution:**

Species Conservation Differential Equation:



In Radial direction (r):

$$\frac{\partial}{\partial t}\left(\rho Y_i 2\pi r\Delta r\right) = \rho_i \overline{u}_{r_i} A\Big|_r - \rho_i \overline{u}_{r_i} A\Big|_{r+\Delta r} - \frac{\rho_i \overline{u}_{r_i}}{r} A\Delta r + \dot{\omega}_i''' 2\pi r\Delta r$$

$$\frac{\partial}{\partial t}\left(\rho Y_i 2\pi r\Delta r\right) = -\Delta r \frac{\partial}{\partial r}\left(\rho_i \overline{u}_{r_i} 2\pi r\right) + \dot{\omega}_i''' 2\pi r\Delta r$$

$$\frac{\partial}{\partial t}\left(\rho Y_i\right) = -\frac{1}{r}\frac{\partial}{\partial r}\left(\rho_i \overline{u}_{r_i} r\right) + \dot{\omega}_i'''$$

We know, $\rho_i = \rho Y_i$ and $u_{r_i} = u_r + V_i$

$$\frac{\partial}{\partial t}\left(\rho Y_i\right) + \frac{1}{r}\left[\frac{\partial}{\partial r}\left(\rho Y_i \overline{u}_r r\right) + \frac{\partial}{\partial r}\left(\rho Y_i V_i r\right)\right] = \dot{\omega}_i'''$$

We can write, $\rho Y_i V_i = -\rho D_i \frac{\partial Y_i}{\partial r}$

$$\frac{\partial}{\partial t}\left(\rho Y_i\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(\rho Y_i \overline{u}_r r\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(-\rho D_i \frac{\partial Y_i}{\partial r} r\right) = \dot{\omega}_i'''$$

$$\frac{\partial}{\partial t}\left(\rho Y_i\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(\rho Y_i \overline{u}_r r\right) - \frac{1}{r}\frac{\partial}{\partial r}\left(\rho D_i \frac{\partial Y_i}{\partial r} r\right) = \dot{\omega}_i'''$$

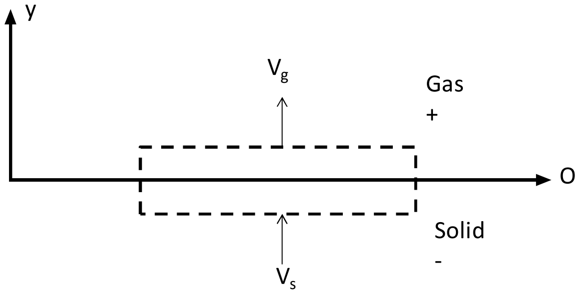
Species Conservation Differential Equation

2. **Solution:**

The continuity equation is given as,

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho v) = 0$$

Integrating above equation in the control volume



$$\oiiint_{\forall} \frac{\partial \rho}{\partial t} d\forall + \oiiint_{\forall} \nabla.[\rho v] d\forall = 0$$

Using divergence theorem, $\oiiint_{\forall} \nabla.\overline{F} d\forall = \oiint_{cs} \overline{F}.d\overline{S}$

$$\oiiint_{\forall} \frac{\partial \rho}{\partial t} d\forall + \oiint_{cs} \rho v.d\overline{S} = 0$$

$$\oiiint_{\forall} \frac{\partial \rho}{\partial t} d\forall + \left[\rho_+ v_+ .\overline{S}_+ \hat{n}_+ - \rho_- v_- .\overline{S}_- \hat{n}_-\right] + \oiint_{\delta A} \rho v.d\overline{S} = 0$$

As, dA →0 => dV→0

Therefore, $\rho_+ v_+ .\overline{S}_+ \hat{n}_+ - \rho_- v_- .\overline{S}_- \hat{n}_- = 0$

$$\rho_g Y_{fg} v_g + \rho_g Y_{ag} v_g + \rho_g Y_{ig} v_g = \rho_s Y_{fs} v_s + \rho_s Y_{as} v_s$$

Now, the species conservation equation for the same control volume

$$\oiiint_{\forall} \frac{\partial}{\partial t} \rho Y_i d\forall + \oiiint_{\forall} \nabla.\rho Y_i \left(\overline{v} + \overline{V}_i\right) d\forall = \oiiint_{\forall} \dot{\omega}_i''' d\forall$$

Using divergence theorem,

$$\oiiint_{\forall} \frac{\partial}{\partial t} \rho Y_i \underbrace{d\forall}_{0} + \oiint_{cs} \nabla.\rho Y_i \left(\overline{v} + \overline{V}_i\right) ds = \oiiint_{\forall} \dot{\omega}_i''' \underbrace{d\forall}_{0}$$

$$-\rho_- Y_{i_-} \left(\overline{v}_- + \overline{V}_{i_-}\right) s_- + \rho_+ Y_{i_+} \left(\overline{v}_+ + \overline{V}_{i_+}\right) s_+ = 0$$

Hence for component (i): $\rho_g Y_{i_g} \left(\overline{v}_g + \overline{V}_{i_g}\right) = 0$

$$\boxed{\rho_g Y_{i_g} \overline{v}_g - \rho_g D_i \left(\frac{\partial Y_{ig}}{\partial x}\right) = 0}$$

Hence for component (f) and (a): $\rho_g Y_{ig}\left(\bar{v}_g + \bar{V}_{ig}\right) - \rho_s Y_{is}\left(\bar{v}_s + \bar{V}_{is}\right) = 0$

$$\rho_g Y_{ig}\bar{v}_g - \rho_g D_i\left(\frac{\partial Y_{ig}}{\partial x}\right) - \rho_s Y_{is}\bar{v}_s = 0$$

$$\boxed{\rho_g Y_{fg}\bar{v}_g - \rho_g D_f\left(\frac{\partial Y_{fg}}{\partial x}\right) - \rho_s Y_{fs}\bar{v}_s = 0}$$

For component f

$$\boxed{\rho_g Y_{ag}\bar{v}_g - \rho_g D_a\left(\frac{\partial Y_{ag}}{\partial x}\right) - \rho_s Y_{as}\bar{v}_s = 0}$$

For component a

3. Solution:

The energy equation is given as:

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial P}{\partial t} + \nabla\left[\rho\bar{U}h + \dot{q}''\right] = \Phi + Q + \rho\sum_{i=1}^{n} Y_i f_i V_i$$

Now assuming adiabatic, inviscid, no body force, we have

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial P}{\partial t} + \nabla\left[\rho\bar{U}h + \dot{q}''\right] = 0$$

Integrating over the control volume,

$$\int_{\forall}\frac{\partial(\rho h)}{\partial t}d\forall - \int_{\forall}\frac{\partial P}{\partial t}d\forall - \int_{\forall}\nabla\left[\rho\bar{U}h + \dot{q}''\right]d\forall = 0$$

Applying divergence theorem,

$$\int_{cv}\nabla\left[\rho\bar{U}h + \dot{q}''\right]ds = 0$$

$$\int_{cv}\left[\rho\bar{U}h - \lambda\frac{dT}{dy} + \sum_{i=1}^{n} h_i Y_i V_i\right]ds = 0$$

Energy Balance at liquid Interface:

$$\rho_+\bar{U}_+h_+ - k_+\left.\frac{dT}{dy}\right|_+ + \rho_+\sum_{i=1}^{n} h_{i+}Y_{i+}V_{i+} = \rho_-\bar{U}_-h_- - \underbrace{k_-\left.\frac{dT}{dy}\right|_-}_{\Downarrow} + \underbrace{\rho_-\sum_{i=1}^{n} h_{i-}Y_{i-}V_{i-}}_{\Downarrow}$$

Pure fuel only & No absorption of outside gases	No temp. gradient inside liquid phase

$$\rho_+\overline{U}_+ = \rho_-\overline{U}_- = \dot{m}''$$
$$h_- = h_{f-}$$

$$\therefore \dot{m}''h_+ - k_+ \left.\frac{dT}{dy}\right|_+ + \rho_+ \sum_{i=1}^{n} h_{i+}Y_{i+}V_{i+} = \dot{m}''h_{f-} \rightarrow (1)$$

$$h_+ = \sum_{i=1}^{n} h_{i+}Y_{i+}$$

Recall Species interface Boundary Conditions:

$$\dot{m}''Y_{i-} = \dot{m}''Y_{i+} + \rho_g Y_{i+}V_{i+}$$

Summing over all ‘i’

$$\sum_{i=1}^{n} \dot{m}''Y_{i-}h_{i-} = \sum_{i=1}^{n} \dot{m}''Y_{i+}h_{i+} + \sum_{i=1}^{n} \rho_g Y_{i+}V_{i+}h_{i+}$$

$$Y_{i-} = \begin{cases} Y_{F-} = 1 \\ Y_i = 0 \\ i \neq F \end{cases}$$

$$\dot{m}''h_{F+} = \dot{m}''h_+ + \sum_{i=1}^{n} \rho_g Y_{i+}V_{i+}h_{i+} \rightarrow (2)$$

Substituting (2) in (1)

$$\dot{m}''h_{F+} - \underbrace{\rho_+ \sum_{i=1}^{n} h_{i+}V_{i+}Y_{i+}}_{0} - k_+ \left.\frac{dT}{dY}\right|_+ + \underbrace{\rho_+ \sum_{i=1}^{n} h_{i+}V_{i+}Y_{i+}}_{0} = \dot{m}''h_{f-}$$

$$\boxed{k_+ \left.\frac{dT}{dy}\right|_+ = k_g \left.\frac{dT}{dy}\right|_g = \dot{m}''\left[h_{f+} - h_{f-}\right] = \dot{m}''\left[h_{fg} - h_{fL}\right] = \dot{m}''L}$$

4. Solution:

Given, $T = 300K \qquad P = 1atm = 101325Pa$

$\sigma_{H_2} = 2.827 \qquad \sigma_{O_2} = 3.467 \qquad \sigma_{CH_4} = 3.758$

$\frac{\varepsilon_{H_2}}{\kappa_B} = 59.7 \qquad \frac{\varepsilon_{O_2}}{\kappa_B} = 106.7 \qquad \frac{\varepsilon_{CH_2}}{\kappa_B} = 148.6$

$$D_{AB} = \frac{0.0266T^{3/2}}{P(MW_{AB})^{1/2}\sigma_{AB}^2\Omega_D} \qquad MW_{AB} = 2\left[\frac{1}{MW_{H_2}} + \frac{1}{MW_{O_2}}\right]^{-1}$$

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} \qquad \Omega_D = \frac{A}{(T^*)^B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)}$$

$A = 1.06036 \qquad C = 0.19300 \qquad E = 1.03587 \qquad G = 1.76474$

$B = 0.15610 \qquad D = 0.47365 \qquad F = 1.52996 \qquad H = 3.89411$

$$T^* = \frac{\kappa_B T}{\varepsilon_{AB}} = \frac{\kappa_B T}{(\varepsilon_A \varepsilon_B)^{1/2}}$$

a) Binary diffusivity of Hydrogen in Oxygen

$$MW_{AB} = 2\left[\frac{1}{MW_{H_2}} + \frac{1}{MW_{O_2}}\right]^{-1} = 2\left[\frac{1}{2} + \frac{1}{32}\right]^{-1} = 3.7647$$

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{2.827 + 3.467}{2} = 3.147$$

$$T^* = \frac{\kappa_B T}{\varepsilon_{AB}} = \frac{\kappa_B T}{(\varepsilon_A \varepsilon_B)^{1/2}} = \frac{\kappa_B T}{(\varepsilon_{H_2}\varepsilon_{O_2})^{1/2}} = \frac{300 \times \kappa_B}{(59.7\kappa_B \times 106.7\kappa_B)^{1/2}} = 3.7588$$

$$\Omega_D = \frac{A}{(T^*)^B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)}$$

$$\Omega_D = \frac{1.06036}{(3.7588)^{0.15610}} + \frac{0.19300}{\exp(0.47365 \times 3.7588)} + \frac{1.03587}{\exp(1.52996 \times 3.7588)} + \frac{1.76474}{\exp(3.89411 \times 3.7588)}$$

$$\Omega_D = 0.89746$$

$$D_{AB} = \frac{0.0266T^{3/2}}{P(MW_{AB})^{1/2}\sigma_{AB}^2\Omega_D} = \frac{0.0266 \times 300^{3/2}}{101325 \times (3.7647)^{1/2} \times 3.147^2 \times 0.89746} = 7.9099 \times 10^{-5}$$

$$D_{H_2-O_2} = 7.9099 \times 10^{-5}$$

b) Binary diffusivity of Methane in Oxygen

$$MW_{AB} = 2\left[\frac{1}{MW_{CH_4}} + \frac{1}{MW_{O_2}}\right]^{-1} = 2\left[\frac{1}{16} + \frac{1}{32}\right]^{-1} = 21.3333$$

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{3.758 + 3.467}{2} = 3.6125$$

$$T^* = \frac{\kappa_B T}{\varepsilon_{AB}} = \frac{\kappa_B T}{(\varepsilon_A \varepsilon_B)^{1/2}} = \frac{\kappa_B T}{(\varepsilon_{CH_4} \varepsilon_{O_2})^{1/2}} = \frac{300 \times \kappa_B}{(148.6\kappa_B \times 106.7\kappa_B)^{1/2}} = 2.3824$$

$$\Omega_D = \frac{A}{(T^*)^B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)}$$

$$\Omega_D = \frac{1.06036}{(2.3824)^{0.15610}} + \frac{0.19300}{\exp(0.47365 \times 2.3824)} + \frac{1.03587}{\exp(1.52996 \times 2.3824)} + \frac{1.76474}{\exp(3.89411 \times 2.3824)}$$

$$\Omega_D = 1.01564$$

$$D_{AB} = \frac{0.0266T^{3/2}}{P(MW_{AB})^{1/2}\sigma_{AB}^2\Omega_D} = \frac{0.0266 \times 300^{3/2}}{101325 \times (22.3333)^{1/2} \times 3.6125^2 \times 1.01564} = 2.2282 \times 10^{-5}$$

$$D_{CH_4-O_2} = 2.2282 \times 10^{-5}$$