Governing Equations for the Computation of Counterflow Flames

Continuity equation in cylindrical coordinates (x, r)

$$\frac{\partial}{\partial x}(\rho u)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho v)=0 \qquad (3.1)$$

Note that the flow variables such as u, ρ , T, Y_k etc. are only functions of x,. The above equation can be written as

$$\frac{1}{r}\frac{\partial}{\partial r}(vr)=-\frac{1}{\rho}\frac{\partial}{\partial x}(\rho u)=2F(x) \qquad (3.2)$$

Integrating (3.2), we have

$$v=F(x)\cdot r \qquad (3.3)$$

Then

$$\frac{\partial v}{\partial r}=F(x)=\frac{v}{r} \qquad (3.4)$$

Substituting (3.2) and (3.4) in (3.1)

$$\frac{\partial}{\partial x}(\rho u)+2\rho\frac{v}{r}=0 \qquad (3.5)$$

We define

$$U(x)=\frac{\rho u}{2} \qquad (3.6)$$

$$G(x)=-\frac{\rho v}{r} \qquad (3.7)$$

which are function of x only. Substituting in (3.5) we have

$$G(x)=\frac{dU(x)}{dx} \qquad (3.8)$$

From (3.7) and (3.8) we have

$$v=-\frac{r}{\rho}\frac{dU}{dx} \qquad (3.9)$$

$$\frac{\partial v}{\partial x}=-r\frac{d}{dx}\left(\frac{1}{\rho}\frac{dU}{dx}\right) \qquad (3.10)$$

Momentum conservation equations

Axial momentum equation using cylindrical coordinates

$$\rho \frac{Du}{Dt} = -\frac{\partial p}{\partial x} + \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\tau_{rx} \right) + \frac{\partial \tau_{xx}}{\partial x} \right) \tag{3.11}$$

where τ are expressed as

$$\tau_{rx} = \mu\left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right) \tag{3.12}$$

$$\tau_{xx} = \mu\left(2\frac{\partial u}{\partial x} - \frac{2}{3}\left(\nabla \cdot \vec{\mathbf{v}} \right) \right) \tag{3.13}$$

Substituting and considering steady flow with u = u(x) and μ = μ (x)

$$\rho u \frac{du}{dx} = -\frac{\partial p}{\partial x} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial x}\left[\mu\left(2\frac{du}{dx} - \frac{2}{3}\left(\nabla \cdot \vec{\mathbf{v}} \right) \right) \right] \tag{3.14}$$

Recalling (3.6) and developing derivatives

$$4U\frac{d}{dx}\left(\frac{U}{\rho} \right) = -\frac{\partial p}{\partial x} + \mu\left(\frac{1}{r}\frac{\partial v}{\partial x} + \frac{\partial^2 v}{\partial x \partial r} \right) + \frac{\partial}{\partial x}\left[\mu\left(2\frac{du}{dx} - \frac{2}{3}\frac{du}{dx} - \frac{2}{3}\frac{1}{r}\frac{\partial (vr)}{\partial r} \right) \right] \tag{3.15}$$

From (3.4):

$$\frac{\partial p}{\partial x} = -4U\frac{d}{dx}\left(\frac{U}{\rho} \right) + \frac{2\mu}{r}\frac{\partial v}{\partial x} + \frac{\partial}{\partial x}\left[\mu\left(\frac{4}{3}\frac{du}{dx} - \frac{4}{3}\frac{v}{r} \right) \right] \tag{3.16}$$

Recalling (3.6), (3.12) and (3.13) we get

$$\frac{\partial p}{\partial x} = -4U\frac{d}{dx}\left(\frac{U}{\rho} \right) - 2\mu\frac{d}{dx}\left(\frac{1}{\rho}\frac{dU}{dx} \right) + \frac{4}{3}\frac{d}{dx}\left[2\mu\frac{d}{dx}\left(\frac{U}{\rho} \right) + \frac{\mu}{\rho}\frac{dU}{dx} \right] \tag{3.17}$$

Radial momentum equation

$$\rho \frac{Dv}{Dt} = -\frac{\partial p}{\partial r} + \left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\tau_{rr} \right) - \frac{\tau_{\theta\theta}}{r} + \frac{\partial \tau_{rx}}{\partial x} \right) \tag{3.18}$$

Expressing τ_{rr}, $\tau_{\theta\theta}$, and τ_{rx} and substituting we get (3.22)

$$\tau_{rr} = \mu\left(2\frac{\partial v}{\partial r} - \frac{2}{3}\left(\nabla \cdot \vec{\mathbf{v}} \right) \right) \tag{3.19}$$

$$\tau_{\theta\theta} = \mu\left(2\frac{v}{r} - \frac{2}{3}\left(\nabla \cdot \vec{\mathbf{v}} \right) \right) \tag{3.20}$$

$$\tau_{rx} = \mu\left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right) \tag{3.21}$$

$$\boldsymbol{r}\left(u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial r}\right)=$$

$$-\frac{\partial p}{\partial r}+\frac{1}{r}\frac{\partial}{\partial r}\left(rm\left(2\frac{\partial v}{\partial r}-\frac{2}{3}(\nabla\cdot\vec{\mathbf{v}})\right)\right)-\frac{m}{r}\left(2\frac{v}{r}-\frac{2}{3}(\nabla\cdot\vec{\mathbf{v}})\right)+\frac{\partial}{\partial x}\left(m\frac{\partial v}{\partial x}\right) \qquad (3.22)$$

Since $\frac{v}{r}$ and divergence of velocity, $\nabla\cdot\vec{\mathbf{v}}=\frac{du}{dx}+2\frac{v}{r}$, are functions of x only, we get:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rm\left(2\frac{\partial v}{\partial r}-\frac{2}{3}(\nabla\cdot\vec{\mathbf{v}})\right)\right)=\frac{m}{r}\left(2\frac{\partial v}{\partial r}-\frac{2}{3}(\nabla\cdot\vec{\mathbf{v}})\right) \qquad (3.23)$$

Substituting (3.23) in (3.22) and simplifying:

$$\frac{\partial p}{\partial r}=2U\frac{\partial}{\partial x}\left(\frac{r}{\boldsymbol{r}}\frac{dU}{dx}\right)-\frac{v^2\boldsymbol{r}}{r}-r\frac{d}{dx}\left(m\frac{d}{dx}\left(\frac{1}{\boldsymbol{r}}\frac{dU}{dx}\right)\right) \qquad (3.24)$$

Adding and subtracting $\left(\frac{r}{\boldsymbol{r}}\frac{dU}{dx}\right)\frac{d(2U)}{dx}$, substituting for v, and rearranging we have

$$\frac{\partial p}{\partial r}=r\frac{d}{dx}\left(\frac{2U}{\boldsymbol{r}}\frac{dU}{dx}\right)-2\frac{r}{\boldsymbol{r}}\left(\frac{dU}{dx}\right)^2-\frac{r}{\boldsymbol{r}}\left(\frac{dU}{dx}\right)^2-r\frac{d}{dx}\left(m\frac{d}{dx}\left(\frac{1}{\boldsymbol{r}}\frac{dU}{dx}\right)\right) \qquad (3.26)$$

Dividing for r we get

$$\frac{1}{r}\frac{\partial p}{\partial r}=\frac{d}{dx}\left(\frac{2U}{\boldsymbol{r}}\frac{dU}{dx}\right)-\frac{3}{\boldsymbol{r}}\left(\frac{dU}{dx}\right)^2-\frac{d}{dx}\left(m\frac{d}{dx}\left(\frac{1}{\boldsymbol{r}}\frac{dU}{dx}\right)\right) \qquad (3.27)$$

From (3.17) and (3.27) we observe that $\frac{1}{r}\left(\frac{\partial p}{\partial r}\right)$ and $\frac{\partial p}{\partial x}$ are function of x only. Thus

$$\frac{\partial}{\partial x}\left(\frac{1}{r}\frac{\partial p}{\partial r}\right)=\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{\partial p}{\partial x}\right)=0 \qquad (3.28)$$

It follows

$$\frac{1}{r}\left(\frac{\partial p}{\partial r}\right)=H=\cos t \qquad (3.29)$$

H is an eigenvalue of the system.

Using (3.8) and (3.29), we can write (3.27), which is function of x only, i.e.,

$$\frac{d}{dx}\left[m\frac{d}{dx}\left(\frac{G}{r}\right)\right]-2\frac{d}{dx}\left(\frac{UG}{r}\right)+\frac{3}{r}G^{2}+H=0 \qquad (3.30)$$

which is the radial momentum equation. The axial momentum is simply expressed as $\frac{\partial p}{\partial x}=0$

Mass conservation for species *k*

Since composition varies in x direction only, mass conservation equations for species *k* (*k*=1,*K*) can be written as:

$$2U\frac{dY_k}{dx}+\frac{d}{dx}\left(r Y_k v_{k,diff}\right)-\dot{w}_k M_k=0 \qquad (3.31)$$

where Y_k, V_k, $\dot{w}_k$ W_k *are* mass fraction, diffusion velocity, reaction rate (Kmol/m^3/s) and molecular weight of species *k*.

Energy conservation equation

Since temperature is function of *x* only, the energy equation can be written as

$$2U\frac{dT}{dx}-\frac{1}{c_p}\frac{d}{dx}\left(l\frac{dT}{dx}\right)+\frac{r}{c_p}\sum_k Y_k V_k c_{pk}\frac{dT}{dx}+\frac{1}{c_p}\sum_k h_k \dot{w}_k M_k+\frac{q^R}{c_p}=0 \qquad (3.32)$$

where l is mixture, thermal conductity, q^R represents the radiative heat transport, and h_k is the enthalpy (enthaply of formation plus sensible enthalpy) of species k.

The flame structure is computed by solving the above equations numerically. For the numerical solution, the following boundary conditions are generally employed.

At the Fuel Nozzle (x=0)

$$U=\frac{r_C u_C}{2}, \qquad G=0, \qquad T=T_C, \qquad r u Y_k + r Y_k v_{k,diff}=\left(r u Y_k\right)_C$$

At the Oxidizer Nozzle (x=L)

$$U=\frac{r_O u_O}{2}, \qquad G=0, \qquad T=T_O, \qquad r u Y_k + r Y_k v_{k,diff}=\left(r u Y_k\right)_O$$