Derivation for Homogenous Reacting Gas Mixture in Closed System

An adiabatic system with volume as a function of time, simulating a HCCI engine

Species Equation

$$\dot{\omega}_k = \frac{dc_k}{dt} \qquad \frac{dm_k}{dt} = V\dot{\omega}_k W_k$$

$$v = \frac{V}{m_{tot}} = \frac{1}{\rho} \qquad Y_k = \frac{m_k}{m_{tot}}$$

$$\frac{dY_k}{dt} = v\dot{\omega}_k W_k$$

Energy Equation

$$\frac{du}{dt} + p\frac{dv}{dt} = 0$$

$$u = \sum Y_k u_k \qquad \frac{du}{dt} = \sum Y_k \frac{du_k}{dt} + \sum u_k \frac{dY_k}{dt}$$

$$\frac{du_k}{dt} = c_{v,k}\frac{dT}{dt} \qquad c_v = \sum Y_k c_{v,k}$$

$$\sum Y_k c_{v,k}\frac{dT}{dt} + \sum u_k \frac{dY_k}{dt} + p\frac{dv}{dt} = 0$$

$$c_v\frac{dT}{dt} + p\frac{dv}{dt} + \sum u_k \frac{dY_k}{dt} = 0$$

$$c_v\frac{dT}{dt} + p\frac{dv}{dt} + v\sum u_k \dot{\omega}_k W_k = 0$$

$$\frac{dT}{dt} = -\frac{p\frac{dv}{dt} + v\sum u_k \dot{\omega}_k W_k}{c_v}$$

Pressure Equation from Ideal Gas Law

$$pv = RT$$

$$v\frac{dp}{dt} + p\frac{dv}{dt} = R\frac{dT}{dt} + T\frac{dR}{dt}$$

$$\frac{dp}{dt} = \left(R\frac{dT}{dt} + T\frac{dR}{dt}\right) * \rho$$

$$R = \frac{R_u}{W_{ave}} \qquad W_{ave} = \frac{1}{\sum \frac{Y_k}{W_k}}$$

$$R = R_u * \sum \frac{Y_k}{W_k}$$

$$\frac{dR}{dt} = R_u * \sum \frac{1}{W_k}\frac{dY_k}{dt}$$

$$\frac{dp}{dt} = \left(\frac{R_u}{W_{ave}}\frac{dT}{dt} + TR_u * \sum \frac{1}{W_k}\frac{dY_k}{dt}\right) * \rho$$

Volume Equation

$R = V_{max} / V_{min}$ = compression ratio

f = rotation frequency

ω = 2πf = angular velocity

$$V = V_{ave} + (V_{max} - V_{ave}) * \cos(\omega t)$$

$$V_{ave} = \frac{V_{max} + V_{min}}{2} = \frac{V_{max} + V_{max}/R}{2} = V_{max}\left(\frac{1}{2} + \frac{1}{2R}\right)$$

$$V = V_{max}\left(\frac{1}{2} + \frac{1}{2R}\right) + \left(V_{max} - V_{max}\left(\frac{1}{2} + \frac{1}{2R}\right)\right) * \cos(\omega t)$$

$$V = V_{max}\left(\left(\frac{1}{2} + \frac{1}{2R}\right) + \left(\frac{1}{2} - \frac{1}{2R}\right) * \cos(\omega t)\right)$$

$$V = V_{max}\left(\frac{1}{2} + \frac{1}{2R}\right)\left(1 + \frac{\left(\frac{1}{2} - \frac{1}{2R}\right)}{\left(\frac{1}{2} + \frac{1}{2R}\right)} * \cos(\omega t)\right)$$

$$V = V_{ave}\left(1 + \left(\frac{2}{R+1} - 1\right) * \cos(\omega t)\right)$$

$$R = \frac{V_{max}}{V_{min}} = \frac{1+\alpha}{1-\alpha}$$

$$R - R\alpha = 1 + \alpha \qquad R - 1 = (R+1)\alpha$$

$$\alpha = \frac{R-1}{R+1}$$

$$\frac{2}{R+1} - 1 = \frac{R-1}{R+1} = \alpha$$

$$V = V_{ave}(1 + \alpha\cos(\omega t))$$

$$V_{ave} = \frac{V_{max} + V_{max}\frac{1-\alpha}{1+\alpha}}{2} = V_{max}\left(\frac{1 + \frac{1-\alpha}{1+\alpha}}{2}\right) = \frac{V_{max}}{1+\alpha}$$

$$V = \frac{V_{max}}{1+\alpha}(1 + \alpha\cos(\omega t))$$

Total mass must be constant, the system is closed and no nuclear reactions, therefore I can convert volume to specific volume

$$v = \frac{v_{max}}{1+\alpha}(1 + \alpha\cos(\omega t))$$

$$v_{max} = v_0 = \frac{R_u T_0}{p_0 W_{ave}}$$

$$\frac{dv}{dt} = \frac{v_0}{1+\alpha}(-\alpha\omega\sin(\omega t))$$