1 Equations

1.1 Mass Conservation

$$\frac{dm}{dt} = \sum_{in} \dot{m}_{in} - \sum_{out} \dot{m}_{out} + \dot{m}_{wall}$$

1.2 Species Conservation

$$m\frac{dY_k}{dt} = \sum_{in} \dot{m_{in}}(Y_{k,in} - Y_k) - \sum_{out} \dot{m}_{out} Y_k + V\dot{\omega}_k W_k$$

1.3 Energy Conservation

$$mc_v\frac{dT}{dt} = -p\frac{dV}{dt} - \dot{Q} + \sum_{in} \dot{m_{in}} \left(h_{in} - \sum_k u_k Y_{k,in} \right) - \frac{pV}{m} \sum_{out} \dot{m}_{out} - \sum_k V\dot{\omega}_k W_k u_k$$

$$c_v = 2.5R \sum_k \frac{Y_k}{W_k}$$

1.4 Chemical Reactions

$$\sum_{k=1}^{N} \nu'_{kj} \mathcal{M}_k \leftrightharpoons \sum_{k=1}^{N} \nu''_{kj} \mathcal{M}_k, \sum_{k=1}^{N} \nu'_{kj} W_k = \sum_{k=1}^{N} \nu''_{kj} W_k, \nu_{kj} = \nu''_{kj} - \nu'_{kj}$$

$$\dot{\omega}_k = \sum_{j=1}^{M} \dot{\omega}_{kj} = W_k \sum_{j=1}^{M} \nu_{kj} \mathcal{Q}_j$$

$$p = \rho \frac{R}{W} T = \rho \sum_k \frac{Y_k}{W_k} T, \rho = \frac{m}{V}$$

$$\mathcal{Q}_j = K_{fj} \prod_{k=1}^{N} [X_k]^{\nu'_{kj}} - K_{rj} \prod_{k=1}^{N} [X_k]^{\nu''_{kj}}, [X_k] = \frac{\rho Y_k}{W_k}$$

$$K_{fj} = A_{fj} T^{\beta_j} \exp\left(-\frac{E_j}{RT} \right), K_{rj} = \frac{K_{fj}}{\left(\frac{p_a}{RT}\right)^{\sum_{k=1}^{N} \nu_{kj}} \exp\left(\frac{\Delta S_j^0}{R} - \frac{\Delta H_j^0}{RT} \right)}$$

2 Variables

The known quantities are:

$$\dot{m}_{in}, \dot{m}_{out}, \dot{m}_{wall}, h_{in}, \dot{Q}, V, W_k, c_v, u_k, Y_{in}, R, p_a, \Delta S_j^0, \Delta H_j^0$$

The model parameters are:

$$A_{fj}, \beta_j, E_j$$

The unknowns in our systems of ODEs are:

$$m, Y, T$$

3 System of ODEs

Combining equations together, we have

$$\dot{m} = h(t)$$

$$\dot{Y} = f(Y, T)$$

$$\dot{T} = g(Y, T)$$