

Derivation for time dependent gas mixture in a perfectly stirred reactor with an open system

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My assumptions are: ignore surface reactions, heat loss

* = in

\dot{m} = outlet mass flow rate

\dot{m}^* = inlet mass flow rate

ρ = mass density

V = reactor volume

T = gas temperature

$\tau = m/\dot{m}^*$ = residence time

Mass conservation

$$\frac{dm}{dt} = \frac{d(\rho V)}{dt} = \dot{m}^* - \dot{m}$$

$$V \frac{d\rho}{dt} = \frac{\rho V}{\tau} - \dot{m}$$

$$\dot{m} = \frac{\rho V}{\tau} - V \frac{d\rho}{dt}$$

Species equation

$$\frac{dm_i}{dt} = \frac{d(\rho V Y_i)}{dt} = \dot{m}^* Y_i^* - \dot{m} Y_i + \dot{\omega}_i W_i V = \rho V \frac{dY_i}{dt} + Y_i \frac{d(\rho V)}{dt}$$

$$\rho V \frac{dY_i}{dt} = \dot{m}^* Y_i^* - \dot{m} Y_i + \dot{\omega}_i W_i V - Y_i \frac{d(\rho V)}{dt}$$

Substitute continuity

$$\rho V \frac{dY_i}{dt} = \dot{m}^* Y_i^* - \left(\dot{m}^* - \frac{d(\rho V)}{dt} \right) Y_i + \dot{\omega}_i W_i V - Y_i \frac{d(\rho V)}{dt}$$

Expand terms

$$\rho V \frac{dY_i}{dt} = \dot{m}^* Y_i^* - \dot{m}^* Y_i + \frac{d(\rho V)}{dt} Y_i + \dot{\omega}_i W_i V - Y_i \frac{d(\rho V)}{dt}$$

Cancel terms

$$\rho V \frac{dY_i}{dt} = \dot{m}^* Y_i^* - \dot{m}^* Y_i + \dot{\omega}_i W_i V$$

Which simplifies to

$$\frac{dY_i}{dt} = \frac{1}{\tau} (Y_i^* - Y_i) + \frac{\dot{\omega}_i W_i}{\rho}$$

Where

$$\tau = \frac{\rho V}{\dot{m}^*}$$

Energy Equation

This reactor is constant pressure, but even though there is a constant total volume there is not constant specific volume

$$\frac{du}{dt} = \dot{q}_{net,in} - p \frac{dv}{dt}$$

Definition of enthalpy

$$h \equiv u + pv$$

$$\frac{dh}{dt} = \frac{du}{dt} + p \frac{dv}{dt} + v \frac{dp}{dt}$$

$\frac{dp}{dt} = 0$ because constant pressure, substitute $\frac{du}{dt}$ equation into $\frac{dh}{dt}$ equation $p \frac{dv}{dt}$ terms cancel

$$\frac{dh}{dt} = \dot{q}_{net,in}$$

Therefore we can conserve enthalpy instead of energy, energy is still conserved but would need an additional equation from ideal gas law to calculate $\frac{dv}{dt}$ if we would want to conserve energy instead of enthalpy.

$$\frac{dH}{dt} = \frac{d(\sum m_i h_i)}{dt} = \dot{H}_{in} - \dot{H}_{out}$$

$$\frac{dH}{dt} = \sum m_i \frac{dh_i}{dt} + \sum h_i \frac{dm_i}{dt}$$

$$\frac{dH}{dt} = \sum \rho V Y_i c_p \frac{dT}{dt} + \sum h_i \frac{d(\rho V Y_i)}{dt}$$

$$\frac{dH}{dt} = \frac{dT}{dt} \rho V c_p + \sum h_i \left(Y_i \frac{d(\rho V)}{dt} + \rho V \frac{dY_i}{dt} \right) = \dot{m}^* \sum Y_i^* h_i^* - \dot{m} \sum Y_i h_i$$

$$\frac{dT}{dt} \rho V c_p = \dot{m}^* \sum Y_i^* h_i^* - \dot{m} \sum Y_i h_i - \sum h_i \left(Y_i V \frac{d\rho}{dt} + \rho V \frac{dY_i}{dt} \right)$$

Substitute continuity

$$\frac{dT}{dt} \rho V c_p = \dot{m}^* \sum Y_i^* h_i^* - \left(\frac{\rho V}{\tau} - V \frac{d\rho}{dt} \right) \sum Y_i h_i - \sum h_i \left(Y_i V \frac{d\rho}{dt} + \rho V \frac{dY_i}{dt} \right)$$

Expand terms

$$\frac{dT}{dt} \rho V c_p = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum Y_i h_i + V \frac{d\rho}{dt} \sum Y_i h_i - \frac{d\rho}{dt} V \sum h_i Y_i - \rho V \sum h_i \frac{dY_i}{dt}$$

Cancel terms

$$\frac{dT}{dt} \rho V c_p = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum Y_i h_i - \rho V \sum h_i \frac{dY_i}{dt}$$

Substitute species equation

$$\frac{dT}{dt} \rho V c_p = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum Y_i h_i - \rho V \sum h_i \left(\frac{1}{\tau} (Y_i^* - Y_i) + \frac{\dot{\omega}_i W_i}{\rho} \right)$$

Expand terms

$$\frac{dT}{dt} \rho V c_p = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum Y_i h_i - \frac{\rho V}{\tau} \sum h_i Y_i^* + \frac{\rho V}{\tau} \sum h_i Y_i - V \sum h_i \dot{\omega}_i W_i$$

Cancel terms

$$\frac{dT}{dt} \rho V c_p = \dot{m}^* \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum h_i Y_i^* - V \sum h_i \dot{\omega}_i W_i$$

Substitute $\dot{m}^* = \frac{\rho V}{\tau}$

$$\frac{dT}{dt} \rho V c_p = \frac{\rho V}{\tau} \sum Y_i^* h_i^* - \frac{\rho V}{\tau} \sum h_i Y_i^* - V \sum h_i \dot{\omega}_i W_i$$

$$\frac{dT}{dt} \rho c_p = \frac{\rho}{\tau} \sum Y_i^* (h_i^* - h_i) - \sum h_i \dot{\omega}_i W_i$$

$$\frac{dT}{dt} = \frac{1}{\tau c_p} \sum Y_i^* (h_i^* - h_i) - \frac{1}{\rho c_p} \sum h_i \dot{\omega}_i W_i$$

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