

# Derivation for Time Dependent Gas Mixture in a Perfectly Stirred Reactor

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# Derivation for Time Dependent Gas Mixture in a Perfectly Stirred Reactor

An open system with constant pressure and volume, assumptions: ignore surface reactions and heat loss

\* = in  
 $\dot{m}$  = outlet mass flow rate  
 $\dot{m}^*$  = inlet mass flow rate  
 $\rho$  = mass density  
 $V$  = reactor volume  
 $T$  = gas temperature  
 $\tau = m/\dot{m}^* = \text{residence time}$

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

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

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

Energy Equation, specific volume not constant

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

$$h \equiv u + pv$$

Definition of enthalpy

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

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

$\frac{dh}{dt} = \dot{q}_{net,in}$  We can conserve enthalpy instead of energy, energy is still conserved but would need an additional equation from ideal gas law to calculate  $\frac{dv}{dt}$

$$\frac{dH}{dt} = \frac{d(\sum m_i h_i)}{dt} = \dot{H}_{in} - \dot{H}_{out} \quad \frac{dH}{dt} = \sum m_i \frac{dh_i}{dt} + \sum h_i \frac{dm_i}{dt} \quad \frac{dH}{dt} = \sum \rho V Y_i c_{p,i} \frac{dT}{dt} + \sum h_i \frac{d(\rho V Y_i)}{dt}$$

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

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

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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Version 1.3, 3 November 2008

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