Design of Alternative Energy Systems

Fuel Cell Calculations

**Reaction Equations**
Overall reaction for any hydrocarbon fuel reacting with oxygen in air

(1) hydrocarbon fuel + (a)O₂ + (a)(3.76)N₂ → (b)CO₂ + (c)H₂O + (a)(3.76)N₂

Solve for a, b, and c by balancing carbon, hydrogen, and oxygen

Ion reactions
For hydrogen
Anode: H₂ → 2e⁻ + 2H⁺
Cathode: 2e⁻ + 2H⁺ + ½ O₂ → H₂O

Nₑ = 2 kmoles of electron/kmole of fuel

For hydrocarbon with water
Anode: CₓHᵧOᵢ + (2x-z)H₂O → xCO₂ + (4x+y-2z)H⁺ + (4x+y-2z)e⁻
Cathode: (x+y/4-z/2)O₂ + (4x+y-2z)H⁺ + (4x+y-2z)e⁻ → (2x+y/2-z)H₂O

Nₑ = (4x+y-2z) kmoles of electron/kmole of fuel

**Enthalpy and Entropy Evaluations**
The enthalpy of a reactant or product is taken as

$$ \overline{h}_i = \overline{h}_{f,i} + \Delta \overline{h}_i $$

where

- $\overline{h}_{f,i}$: enthalpy of formation for the compound
- $\Delta \overline{h}_i$: change in enthalpy for the compound as it goes from 298 K and 101 kPa to the fuel cell temperature and pressure

For an ideal gas

$$ \Delta \overline{h}_i = \overline{h}_i(T_{FC}) - \overline{h}_i(298 K) \text{ where the } \overline{h}_i \text{'s are read from the ideal gas table for the compound} $$

If these tables are not available, we could use

$$ \Delta \overline{h}_i = \overline{c}_{P,i}(T_{FC} - 298) \text{ where } \overline{c}_{P,i} \text{ is the molar specific heat for the compound evaluated at the average temperature, } (T_{FC}+298)/2 $$
For an incompressible liquid

$$\Delta\bar{h}_i = \bar{c}_p,i \left( T_{FC} - 298 \right) + \left( P_{FC} - 101 \right) / \bar{\rho}_i$$

where

- $\bar{c}_p,i$ is the molar specific heat for the compound evaluated at the average temperature, $(T_{FC}+298)/2$
- $\bar{\rho}_i$ is the molar density for the compound evaluated at the average temperature, $(T_{FC}+298)/2$

The entropy of a reactant or product for an ideal gas is taken as

$$\bar{s}_i = \bar{s}_i^0 - R_u \ln(y_i)$$

where

- $\bar{s}_i^0$: temperature part of the entropy for the compound, read from the tables
- $R_u$: universal gas constant, 8.314 kJ/(kmole⋅K)
- $y_i$: mole fraction of the compound in the gas mixture

If tables are not available, we could use

$$\bar{s}_i^0 = \bar{s}_i^0 \left( \text{at 298 K} \right) + \bar{c}_p,i \ln(T_{FC}/298)$$

where $\bar{c}_p,i$ is the molar specific heat for the compound evaluated at the average temperature, $(T_{FC}+298)/2$

For an incompressible liquid

$$\bar{s}_i = \bar{s}_i \left( \text{at 298 K} \right) + \bar{c}_p,i \ln(T_{FC}/298)$$

where $\bar{c}_p,i$ is the molar specific heat for the compound evaluated at the average temperature, $(T_{FC}+298)/2$

**Electrical Calculations**

Assuming an isothermal, reversible fuel cell

Specific Electrical Work

$$\bar{w}_{elec} = \sum_{\text{reactants}} v_i \bar{h}_i - \sum_{\text{products}} v_j \bar{h}_j - T_{FC} \left\{ \sum_{\text{reactants}} v_i \bar{s}_i - \sum_{\text{products}} v_j \bar{s}_j \right\}$$

where the $v$’s are the stoichiometric coefficients from the balanced chemical reaction equation.
Ideal Efficiency

\[
\eta_i = 1 - \frac{T_{FC} \left\{ \sum_{\text{reactants}} v_i \bar{s}_i - \sum_{\text{products}} v_j \bar{s}_j \right\}}{\sum_{\text{reactants}} v_i \bar{h}_i - \sum_{\text{products}} v_j \bar{h}_j}
\]

Ideal Voltage

\[
V_i = \frac{W_{\text{elec}}}{(96,487) N_e}
\]

Ideal Current

\[
I_i = \frac{\dot{W}_{\text{elec}}}{V_i}
\]

Required Mass Flow Rate of Fuel

\[
\dot{m}_{\text{fuel}} = \frac{M_{\text{fuel}} \dot{W}_{\text{elec}}}{W_{\text{elec}}}
\]

Number of Fuel Cell Stacks Required

\[
\text{number of stacks} = \frac{V_{\text{required}}}{V_{\text{cell}}}
\]