



Sustainable Energy
**Mod. 6: Fuel Cells & Distributed
Generation Systems**

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Exercise II: fuel cells (advanced calculations)

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Exercise 6: For the above example, determine the composition of the effluent (spent) fuel stream in mol percent including the effect of the water gas shift reaction. Assume an effluent temperature of 1200°F (922 K) and that the water gas shift reaction proceeds to equilibrium.

**Anode outlet without shifting:
(from Exercise 4)**

Mol percent FC outlet
0.00
0.00
50.00
12.50
37.50
100.00

Solution (1/3):

- Water gas shift reaction: $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$
- The double headed arrow is used to indicate that the reaction is in equilibrium (not completely to the left or to the right)
- Equilibrium concentrations can be determined by a temperature dependent equilibrium constant:

$$K = \frac{[\text{CO}_2][\text{H}_2]}{[\text{CO}][\text{H}_2\text{O}]}$$

Solution (2/3):

• Equilibrium constants can be calculated from fundamental chemical data such as Gibbs free energy, or can be determined from temperature dependent tables.

• A formula valid between 1000-1450°F: $K = e^{(4,276/T - 3.961)}$

• So: $K = 1.967$ at 922 K

• A check from composition shows concentrations are not in equilibrium:

$$\frac{[\text{CO}_2][\text{H}_2]}{[\text{CO}][\text{H}_2\text{O}]} = \frac{[0.50][0.125]}{[0.0][0.375]} = \infty \neq 1.967$$

• By introducing a variable x (extent of the reaction):

$$K = \frac{[\text{CO}_2 + x][\text{H}_2 + x]}{[\text{CO} - x][\text{H}_2\text{O} - x]}$$

• It can be: $\underbrace{(1-K)x^2}_a + \underbrace{\{[\text{CO}_2] + [\text{H}_2] + K([\text{CO}] + [\text{H}_2\text{O}])\}}_b x + \underbrace{\{[\text{CO}_2][\text{H}_2] - [\text{CO}][\text{H}_2\text{O}]K\}}_c = 0$

• It is a second order algebraic equation: $ax^2 + bx + c = 0$

• It can be solved: $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

• The solutions are: $x_1 = -0.0445$ and $x_2 = 1.454$

Solution (3/3):

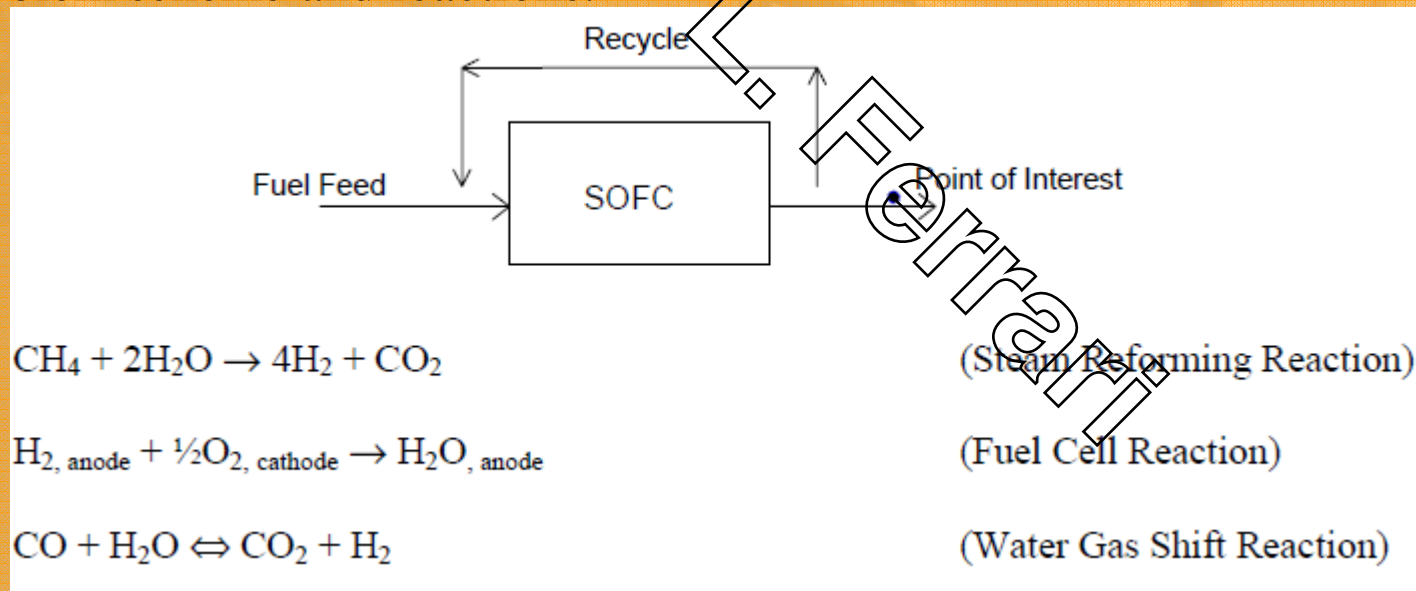
- The larger root is physically impossible; it “wants to” react more CO and H₂O than are initially present.
- The remaining root of -0.0445 is used to compute the equilibrium gas composition, which is shown in the following table.

Gas	mol percent		Lb mol/hr, assuming 100 lb mol/hr basis		Mol percent	
	FC outlet w/o shift.	FC outlet w/o shift	effect of shift rxn	FC outlet in shift equil.	FC outlet in shift equil.	
CO	0.00	0.00	4.45	4.45	4.45	4.45
CO ₂	50.00	50.00	-4.45	45.55	45.55	45.55
H ₂	12.50	12.50	-4.45	8.05	8.05	8.05
H ₂ O	37.50	37.50	4.45	41.95	41.95	41.95
Total	100.0	100.00	0.00	100.00	100.00	100.00

Exercise 7: An SOFC operates at 1800 °F on 100% methane (CH₄) and a fuel utilization of 85%. What is the composition of the effluent (spent) fuel in mol percent? Assume that the methane is completely reformed within the fuel cell, and the moisture required for reforming is supplied by internal recirculation.

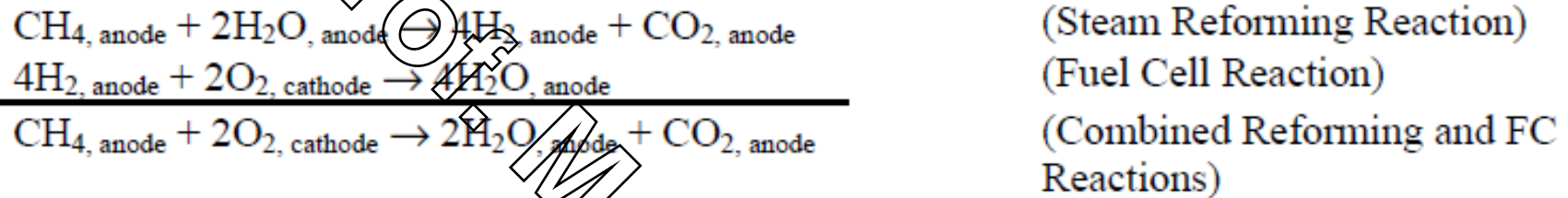
Solution (1/4):

• Problem scheme and reactions:



Solution (2/4):

- Combined reaction for one mole of CH₄:

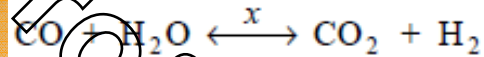


- For ease of calculation, assume a 100 lb/h basis for supplied methane:
- Molecular weight for CH₄: 16.043 lb/lb mol
- Supplied fuel (lb mol/h): $n_{\text{fuel_sup}} = 100/16.043 = 6.23 \text{ lb mol/h}$
- Consumed fuel (lb mol/h): $n_{\text{fuel_cons}} = n_{\text{fuel_sup}} * 0.85 = 5.30 \text{ lb mol/h}$
- The remainder will be reformed but not consumed by the fuel cell reaction.
- Intermediate calculation (no shifting):

Gas	mol percent		lb mol/hr			mol percent	
	FC inlet	FC inlet	Ref / FC rxn	Reforming	FC outlet	FC outlet	FC outlet
CH ₄	100.0	6.23	-5.30	-0.93	0.00	0.00	0.00
CO	0.0	0.00	0.00	0.00	0.00	0.00	0.00
CO ₂	0.0	0.00	5.30	0.93	6.23	33.33	33.33
H ₂	0.0	0.00	0.00	3.74	3.74	20.00	20.00
H ₂ O	0.0	0.00	10.60	-1.87	8.73	46.67	46.67
Total	100.0	6.23	10.60	1.87	18.70	100.00	100.00

Solution (3/4):

- Now apply the water gas shift reaction to determine the true exit composition:



- The equilibrium constant at 1800°F (1255 K): $K = e^{(4276/1255 - 3.961)} = 0.574$
- Coefficient calculation (see Exercise 6):

$$a = (1 - K) = (1 - 0.574) = 0.426$$

$$b = \{[\text{CO}_2] + [\text{H}_2] + K([\text{CO}] + [\text{H}_2\text{O}])\} = 0.3333 + 0.2000 + 0.574 * (0.00 + 0.4667) = 0.8012$$

$$c = \{[\text{CO}_2][\text{H}_2] - [\text{CO}][\text{H}_2\text{O}]K\} = (0.3333)(0.20) - (0.00)(0.4667)(0.574) = 0.0666$$

The result are:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{-0.8012 \pm \sqrt{(0.8012)^2 - 4(0.426)(0.0666)}}{2(0.426)} = -0.0873 \text{ and } -1.794$$

Solution (4/4):

- The only root that is physically possible is $x = -0.0873$.
- The following table summarizes the effect of accounting for the water gas shift equilibrium:

Gas	mol percent		Lb mol/hr, assuming 100 lb mol/hr basis		Mol percent	
	FC outlet w/o shift.	FC outlet w/o shift	Effect of shift rxn	FC outlet in shift equil.	FC outlet in shift equil.	FC outlet in shift equil.
CO	0.00	0.00	-(-8.73)	8.73	8.73	8.73
CO ₂	33.33	33.33	-8.73	24.61	24.61	24.61
H ₂	20.00	20.00	-8.73	11.27	11.27	11.27
H ₂ O	46.67	46.67	-(-8.73)	55.39	55.39	55.39
Total	100.00	100.00	0.00	100.00	100.00	100.00