Energy Conversion & Storage Systems
1399, Semester II, Lecturer: H. Moqtaderi
Problem Set 3
Deadline: 1400/02/12, 14:59

1. Overall reaction of a H_2-Air Fuel cell, can be considered as

$$H_2 + \frac{1}{2}O_2 \rightleftharpoons H_2O$$

and its working temperature is 353 K. Assuming working pressure and species activities are all at standard conditions, calculate LHV (in which assumed all the product water is in the gas phase) and HHV (in which assumed all the product water is in the liquid phase) reversible (open-circuit) voltage by each of the following methods and approximations:

(a) Using the following approximation, that is $\Delta\hat{h}^0$ and $\Delta\hat{s}^0$ are independent of temperature:

$$\Delta\hat{g}(T) \approx \Delta\hat{h}^0 - T\ \Delta\hat{s}^0$$

(b) Assuming constant $\hat{c}_p$ $(\mathrm{kJ/(kmol \cdot K)})$ for each of species, given in the following table:

Chemical Species	c_p (J/mol·K)
O_2	29.4
H_2	28.8
$H_2O_{(g)}$	33.6
$H_2O_{(l)}$	75.4

Hint: You should use the integral form to calculate properties changes.

(c) Using the given polynomials ($R_u = 8.314\ \mathrm{kJ/kmol \cdot K}$) and following table to approximate $\hat{c}_p$ $(\mathrm{kJ/(kmol \cdot K)})$ as a function of temperature. First, define separate Simulink blocks to calculate thermodynamic properties like $\hat{g}$, $\hat{h}$ and $\hat{s}$ based on given inputs: species name and temperature. Then, develop a MATLAB-Simulink model, to predict reversible LHV and HHV voltage.

(d) Develop a MATLAB-Simulink model be capable to compare the results in case (a), (b), and (c) and to report the differences in any other temperature than 353 K.

$$\frac{\hat{c}_p(T)_{H_2}}{R_u} = 3.057 + 2.677 \times 10^{-3}T - 5.810 \times 10^{-6}T^2 + 5.521 \times 10^{-9}T^3 - 1.812 \times 10^{-12}T^4$$

$$\frac{\hat{c}_p(T)_{O_2}}{R_u} = 3.626 - 1.878 \times 10^{-3}T + 7.055 \times 10^{-6}T^2 - 6.764 \times 10^{-9}T^3 + 2.156 \times 10^{-12}T^4$$

$$\frac{\hat{c}_p(T)_{N_2}}{R_u} = 3.675 - 1.208 \times 10^{-3}T + 2.324 \times 10^{-6}T^2 - 0.632 \times 10^{-9}T^3 - 0.226 \times 10^{-12}T^4$$

$$\frac{\hat{c}_p(T)_{Air}}{R_u} = 3.653 - 1.337 \times 10^{-3}T + 3.294 \times 10^{-6}T^2 - 1.913 \times 10^{-9}T^3 + 0.2763 \times 10^{-12}T^4$$

$$\frac{\hat{c}_p(T)_{H_2O}}{R_u} = 4.070 - 1.108 \times 10^{-3}T + 4.152 \times 10^{-6}T^2 - 2.964 \times 10^{-9}T^3 + 0.807 \times 10^{-12}T^4$$

Enthalpy of Formation, Gibbs Energy of Formation, and Entropy Values at 298 K, 1 atm

Species	Molecular Formula	$\bar{h}_f^\circ$ (kJ/kmol)	$\bar{g}_f^\circ$ (kJ/kmol)	$\bar{s}^\circ$ (kJ/kmol · K)
Carbon	C_s	0	0	5.74
Hydrogen	$H_{2,g}$	0	0	130.57
Nitrogen	$N_{2,g}$	0	0	191.50
Oxygen	O_{2g}	0	0	205.03
Carbon monoxide	CO_g	−110,530	−137,150	197.54
Carbon dioxide	$CO_{2,g}$	−393,520	−394,380	213.69
Water vapor	H_2O_g	−241,820	−228,590	188.72
Liquid water	H_2O_l	−285,830	−237,180	69.95
Hydrogen peroxide	$H_2O_{2,g}$	−136,310	−105,600	232.63
Ammonia	$NH_{3,g}$	−46,190	−16,590	192.33
Hydroxyl	OH_g	39,460	34,280	183.75
Methane	$CH_{4,g}$	−74,850	−50,790	186.16
Ethane	$C_2H_{6,g}$	−84,680	−32,890	229.49
Propane	$C_3H_{8,g}$	−103,850	−23,490	269.91
Octane vapor	$C_8H_{18,g}$	−208,450	17,320	463.67
Octane liquid	$C_8H_{18,l}$	−249,910	6,610	360.79
Benzene	$C_6H_{6,g}$	82,930	129,660	269.20
Methanol vapor	CH_3OH_g	−200,890	−162,140	239.70
Methanol liquid	CH_3OH_l	−238,810	−166,290	126.80
Ethanol vapor	$C_2H_5OH_g$	−235,310	−168,570	282.59
Ethanol liquid	$C_2H_5OH_l$	−277,690	−174,890	160.70

2. Given a hydrogen-air fuel cell operating at 353 K. Assume the hydrogen and water vapor mole fractions in the anode are 0.8 and 0.2, respectively, and the oxygen, nitrogen, and water vapor mole fractions in the cathode are 0.15, 0.75, and 0.1, respectively. In addition, the cathode and anode working pressures are 3 and 2 bar, respectively.

   (a) Extend the developed MATLAB-Simulink model in problem 1, to predict LHV and HHV open-circuit (reversible) voltage using the assumption of case (c) in problem 1.

3. Given an H_2–air fuel cell operating at $100\ ^\circ C$ with vapor phase water as the product. Determine the approximate expected change in voltage if air is replaced with oxygen, with all else remaining the same.

4. Chapter 2, problem 5[1].

5. Chapter 2, problem 6[1].

6. Chapter 2, problem 10[1].

7. Chapter 2, problem 11[1].

[1] Ryan O'Hayre, Suk-Won Cha, Whitney G. Colella, Fritz B. Prinz, Fuel Cell Fundamentals, 3rd ed., 2016, John Wiley & Sons.