22CGP070

Clean Energy, Materials and Sustainability

Semester 2 2022/23 | In-Person Exam paper

This examination is to take place in-person at a central University venue under exam conditions. The standard length of time for this paper is **3 hours**.

You will not be able to leave the exam hall for the first 30 or final 15 minutes of your exam. Your invigilator will collect your exam paper when you have finished.

Help during the exam

Invigilators are not able to answer queries about the content of your exam paper. Instead, please make a note of your query in your answer script to be considered during the marking process.

If you feel unwell, please raise your hand so that an invigilator can assist you.

You may use a calculator for this exam. It must comply with the University's Calculator Policy for In-Person exams, in particular that it must not be able to transmit or receive information (e.g., mobile devices and smart watches are **not** allowed).

Attempt **ALL** questions. Each question carries 25 marks.

Candidates should show full working for all calculations and derivations.

An Appendix of constants and conversions is available on the final page of the exam paper.

1. (a) Explain the similarity and two main differences between a fuel cell and a battery.

[3 marks]

(b) Explain why the ionic conductivities of electrolytes are so much lower than the electronic conductivities of metals. [3 marks]

(c) In thermodynamics, define the terms of Internal Energy, Enthalpy and Gibbs Free Energy. [3 marks]

(d) A direct methanol fuel cell (DMFC) operates with a proton-exchange-membrane (PEM) electrolyte at 77°C, the anode is supplied with 1 M methanol (CH_3OH) and the cathode is supplied with 1 atm pure oxygen.

(i) Write and balance the anode half-cell reaction, the cathode half-cell reaction, and the full-cell reaction. Specify the states (gas, liquid or solid) of all reactants and products in these reactions. [3 marks]

(ii) Given the thermodynamic data in Table Q1, and assuming both the enthalpy and entropy are independent of temperature, calculate the reversible thermodynamic efficiency and the reversible cell voltage of this DMFC at 77°C. [6 marks]

Table Q1. Thermodynamic Data.

Chemical Species	**Enthalpy of formation ($kJ\ mol^{-1}$)**	**Entropy ($J\ mol^{-1}\ K^{-1}$)**
CH_3OH (l)	-238.5	127.2
O_2 (g)	0	205.0
CO_2 (g)	-393.5	213.8
H_2O (l)	-285.8	70.0

(iii) Methanol and oxygen are supplied to the DMFC at 0.0015 mol s^{-1} and 0.0055 mol s^{-1}; respectively. If this DMFC generates a current of 700 A at an overvoltage loss of 0.30 V at 77°C, calculate its real efficiency and the amount (in moles) of CO_2 gas produced in 2 hours. [7 marks]

2. (a) Hydrogen fuel and oxygen gas are used in a solid oxide fuel cell running at 700°C. Write and balance the anode half-cell reaction, the cathode half-cell reaction, and the full-cell reaction. Specify the states (gas, liquid or solid) of all reactants and products in these reactions. [3 marks]

(b) If the operating temperature is increased by 50°C, will the reversible thermodynamic efficiency of the hydrogen-oxygen fuel cell increase or decrease? Briefly justify your answer. [3 marks]

(c) A 20 cm^2 proton-exchange membrane fuel cell has the electronic resistance of 0.005 Ω and the ionic (electrolyte) conductivity of 0.100 Ω^{-1} cm^{-1}. If the electrolyte is 50 μm (micro-meter) thick, calculate the ohmic voltage loss for this fuel cell running at the current density of 600 mA cm^{-2}. [4 marks]

(d) In the following electrochemical cell at 298 K shown in the shorthand expression (cell notation) below, write down and balance the oxidation half-cell reaction, the reduction half-cell reaction, and the full-cell reaction. Calculate the electromotive force (EMF) of this cell. Standard Redox Potentials data are shown in Table Q2 that you can choose to use as appropriate. [8 marks]

H_2(g, 1 atm) │ H^+(aq, 0.01M) ‖ Ag^+(aq, 0.1M) │ Ag(s)

Table Q2. Standard Potentials at 298 K.

Half-cell reaction			E^0 (V)
Ag^+(aq) + e^-	$\rightarrow$	Ag(s)	0.80
$2H^+$(aq) + $2e^-$	$\rightarrow$	H_2(g)	0.00

(e) A portable electronic device operates at the voltage of 5.00 V and the current of 6.00 A.

(i) If a single fuel cell delivers a current of 3.00 A at the voltage of 0.50 V, how many of the single fuel cells are required and how are they arranged together to power this portable electronic device? Briefly justify your answer. [3 marks]

(ii) This portable electronic device needs to be operated for 50 hours. Assuming 60% real efficiency of the fuel cells, what is the minimum amount of H_2 fuel (in moles) required? [4 marks]

3. (a) Hydrogen is regarded as a major future energy carrier. Discuss the relative merits as well as challenges of using hydrogen as a fuel. [6 marks]

(b) Reversible thermochemical reaction of MgH_2 given in the equation below has been utilised in energy storage systems. Using the values provided in Table Q3, explain which of the two grades of MgH_2 would be better suited for a MgH_2-fuel cell system. Assume similar absorption kinetics for both grades. [7 marks]

$$MgH_2 + \Delta H \Leftrightarrow Mg + H_2$$

Table Q3. Properties of two grades of Mg-based hydrogen storage materials.

MgH_2 GRADE	**HYDROGEN CAPACITY (WT%)**	**THERMAL CONDUCTIVITY (W $M^{-1}K^{-1}$)**	**ΔH (kJ kg^{-1} MgH_2)**
GRADE A	7.7	10.42	2827
GRADE B	7.7	4.98	2827

(c) Upon investigation of a failed Li-ion battery, large amounts of individual small pieces of Li-containing particles have been identified in the electrolyte. Discuss if this observation could explain possible reasons behind the failure of this battery. [3 marks]

(d) A typical shortcoming of solid-state battery electrolytes is restricted infiltration of the electrolyte into the electrode structure. State three manufacturing methods that could address this problem. [3 marks]

(e) Explain the governing mechanisms responsible for the formation of the dendritic morphology in Li-ion batteries and describe how this morphology grows as a result of Li-ion diffusion. [6 marks]

4. (a) A lithium-ion battery cell has been manufactured using a graphite host C_6Li (CL) and $LiFePO_4$ (LFP) as anode and cathode, respectively. Calculate the gravimetric energy density of the battery system in terms of Wh kg^{-1} operating at an Open Circuit Voltage (OCV) of 3.1 V. Assume the following atomic mass (in amu) values for the different elements: Li:7, C:12, P:32, O:16, Fe:56. [5 marks]

$$C_{max} = \frac{nF}{3.6\ M_w}\ \ [mAh\ g^{-1}]$$

$F=96500$

(b) Discuss the principle of Cradle-to-Grave Life Cycle Assessment (LCA) and compare it to Gate-to-Gate LCA. [5 marks]

(c) One of the most effective approaches to develop more sustainable technologies is to implement the 12 Green Engineering Principles. Briefly discuss the flowing principle: "Output-pulled rather than input-pushed". [5 marks]

(d) A 1000 MWe natural gas power plant is operating continuously over the year on a 55% energy efficiency. The associated CO_2 emission is 0.05 kg/kWhe. A carbon capture process is to be installed on this power plant. The CCS unit can capture 78% of the CO_2 in the exhaust while the energy penalty is 12%.

(i) Calculate how much CO_2 emission can be saved annually. [7 marks]

(ii) Explain what the Effective CO2 Capture Fraction is and calculate the value of the Effective CO_2 Capture Fraction. [3 marks]

END OF PAPER

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APPENDIX
CONSTANTS AND CONVERSIONS

Physical Constants		
Avogadro's number	N_A	6.02×10^{23} atoms/mol
Universal gas constant	R	0.08205 L · atm/mol · K
		8.314 J/mol · K
		83.14 bars · cm^3/mol · K
		8.314 Pa · m^3/mol · K
Planck's constant	h	6.626×10^{-34} J · s
		4.136×10^{-15} eV · s
Boltzmann's constant	k	1.38×10^{-23} J/K
		8.61×10^{-5} eV/K
Electron mass	m_e	9.11×10^{-31} kg
Electron charge	q	1.60×10^{-19} C
Faraday's constant	F	96485.34 C/mol

Conversions	
Weight	2.20 lb = 1 kg
Distance	0.622 mile = 1 km
	3.28×10^{-2} ft = 1 cm
Volume	1000 L = 1 m^3
	0.264 gal = 1 L
	3.53×10^{-2} ft^3 = 1 L

Conversions (cont.)	
Pressure	1.013250×10^5 Pa = 1 atm
	1.013250 bars = 1 atm
	10^5 Pa = 1 bar
	14.7 psi = 1 atm
Energy	6.241506×10^{18} eV = 1 J
	1 calorie = 4.184 J
	9.478134×10^{-4} Btu = 1 J
	2.777778×10^{-7} kWh = 1 J
Power	1 J/s = 1 W
	$1.34 \cdot 10^{-3}$ horsepower = 1 W
	3.415 Btu/h = 1 W