國立臺灣科技大學 109 學年度碩士班招生試題

系所組別：化學工程系碩士班

科　　目：化工熱力學與動力學

(總分為 100 分)

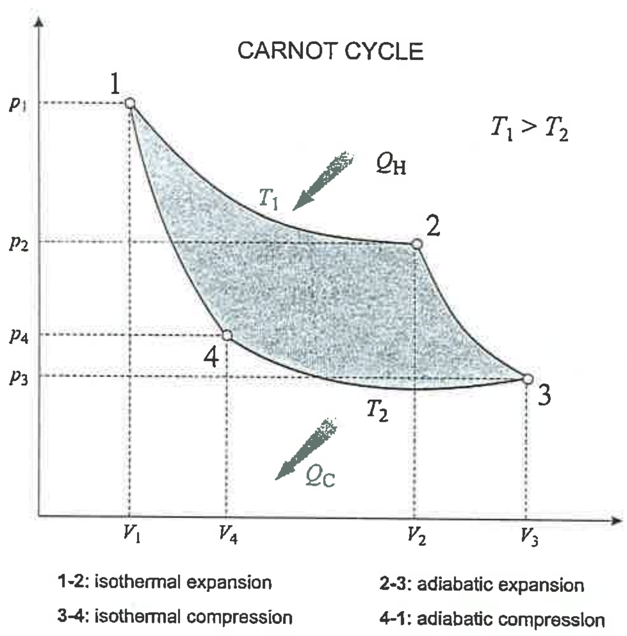
1.

(a) State the energy balance of internal energy (U) in differential change form as a function of the heat (Q) and work (W) for a thermodynamic closed system of one mole ideal gas undergoing a mechanically reversible process. What is the relationship of reversible heat change (dQ_{rev}) with the differential form of entropy (dS)? What is the relationship of reversible work change (dW_{rev}) with the differential form of volume (dV)? (Temperature of the system is T and volume is V) (4 points)

(b) Derive the entropy S at any temperature T and volume V if its initial value is S_0 at temperature T_0 and volume V_0. (Heat capacity at constant volume is C_V, gas constant is R) (6 points)

(c) For isentropic processes (dS = 0) of ideal gases, show the relationship between T and V for two various states, i.e., (T_1, V_1) and (T_2, V_2). (Please use the notation of $\gamma = C_p/C_V$, where C_p is the heat capacity at constant pressure) (6 points)

(d) Sketch the temperature versus entropy diagram (T-S diagram) for a process involving the Carnot's cycle illustrated by the P-V diagram as shown below. Express the heat received from the hot reservoir (Q_H), heat released to the cold reservoir (Q_C), and the work done on the system (W) as functions of temperature and entropy change. What is the total entropy change for the Carnot's cycle? For real heat engine, state two sources of irreversibility that make the total entropy change increasing. (14 points)



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2.

A fuel cell is a device in which a fuel is oxidized electrochemically to produce electric power. The overall reaction for the fuel cell using hydrogen and oxygen as the reactants to form water is as follows.

$$H_{2(g)} + 1/2\ O_{2(g)} \rightarrow H_2O_{(l)}$$

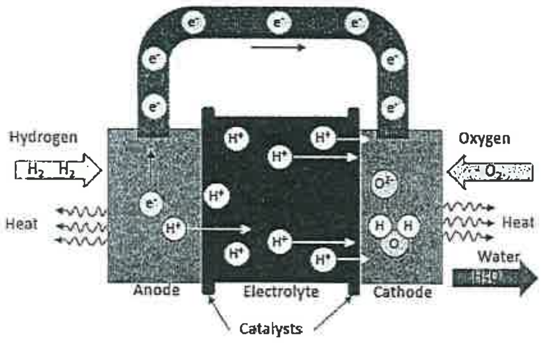

Table Standard heats and free energies of formation and absolute entropies

Name	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)	S° (J/mol·K)
$H_{2(g)}$	0	0	130.5
$O_{2(g)}$	0	0	205
$H_2O_{(l)}$	-285.8	-237.2	69.9

(a) From the above table, give the standard Gibbs free energy change ($\triangle G_{fr}^\circ$) and the standard enthalpy change ($\triangle H_{fr}^\circ$) of reaction. Also calculate the standard entropy change of reaction ($\triangle S_r^\circ$) and show how $\triangle S_r^\circ$ is related with $\triangle G_{fr}^\circ$ and $\triangle H_{fr}^\circ$. (6 points)

(b) What does the standard Gibbs free energy change of reaction means? For a polymer electrolyte fuel cell (PEFC) where the anode reaction is $H_2 \rightarrow 2H^+ + 2e^-$ and cathode reaction is $1/2O_2 + 2e^- \rightarrow O^{2-}$, what is the reversible standard potential (voltage) per mole of hydrogen for the cell reaction? What is the amount of heat emitted from the system per mole of hydrogen? (The Faraday constant is 96500 Coul/mol) (6 points)

(c) A fuel cell vehicle (FCV) using hydrogen as fuel is expected as a clean car and is the first step for the hydrogen energy society. A hydrogen refueling station, which is consist of a compressor, a pressure vessel, a dispenser and so on, is essential infrastructure for FCV. Normally, a fuel cell car needs to be fed with hydrogen up to 70MPa within quite a short time to have enough amount of hydrogen for long moving distances. What would you expect the temperature change for 1 mole of hydrogen originally at 298K and 10MPa to be compressed adiabatically to 70 MPa? Please derive the P-T relation for adiabatic process assuming ideal gas behavior first. What kind of process will you suggest to deal with this hydrogen temperature change? ($\gamma = C_p/C_V = 1.41$ for hydrogen) (8 points)

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3. Based on the general mole balance equation, derive the reactor design equation (in terms of reactor volume (V), molar flow rate of A entering the reactor (F_{A0}), and conversion (X)) for the elementary liquid phase reaction $A \rightarrow B$ carried out in a continuous stirred tank reactor (CSTR) or a plug flow reactor (PFR). (20 points)

4. The elementary liquid phase reaction $A + B \xrightarrow{k} C + D$ is carried out in a reaction system comprising a CSTR (1) and a PFR (2) in series. Size this system provided that $C_{A0} = 0.01$ mol L^{-1}, $C_{B0} = 1$ mol L^{-1}, $v_0 = 1$ L s^{-1}, $F_{A1} = 0.005$ mol s^{-1}, $X_2 = 0.8$ and $k = 0.01$ L mol^{-1} s^{-1}. Note that C_{A0} is the concentration of A entering CSTR (1), C_{B0} is the concentration of B entering CSTR (1), v_0 is the volumetric flow rate entering CSTR (1), F_{A1} is the molar flow rate of A entering PFR (2), X_2 is the conversion at the exit of PFR (2) and k is the reaction rate constant. (20 points)

5. Derive an expression for the equilibrium conversion (X_e) for the following elementary reaction

$A_{(l)} \Longleftrightarrow B_{(l)} + C_{(l)}$. (10 points)