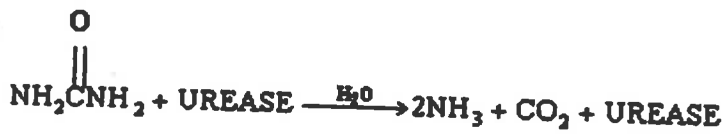
國立臺灣科技大學112學年度碩士班招生試題
系所組別：化學工程系碩士班
科　　目：化工熱力學與動力學

（總分為100分；所有試題務必於答案卷內頁依序作答，否則不予計分）

1. **(10%)** A CSTR is running an isothemal and first order elementary reaction in liquid-phase, A→B. Show that the convergence $x=\dfrac{\tau A e^{\frac{-Ea}{RT}}}{1+\tau A e^{\frac{-Ea}{RT}}}$, when τ is the space time (i.e. V/v_0).

2. **(20%)** The metabolism of urea (NH_2CONH_2) with the enzyme urease can be described in the following reaction,



The rate of reaction is given as a function of urea concentration as the following table. Please determine the rate law of the reaction.

C_{urea} (kmol/m^3)	0.2	0.02	0.01	0.005	0.002
$-r_{urea}$ (kmol/m^3.s)	1.08	0.55	0.38	0.2	0.09

3. **(20%)** Table 1 summarizes the data of $C_{A0}/-r_A$ versus X_A for a nonisothermal, nonelementary, multiple-reaction liquid phase decomposition of reactant A. Volumetric flow rate is 40L/min. Please analysis the following questions and use Simpson's rule to evaluate any integrals in your calculation

Table 1

$C_{A0}/-r_A$ (min)	15	20	40	60	45	25	10	15	40	70
X_A	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9

Simpson's rule: $\int_{X0}^{X2} f(x)dx=\frac{\Delta X}{3}[f(X_0)+4f(X_1)+f(X_2)]$

(a) Consider a CSTR and a PFR are connected in series. The intermediate conversion is 0.4 and the final conversion is 0.8. How should the reactors be arranged to obtain the minimum total reactor volume? (10%)

(b) If using two reactors in series, is there a better means (i.e. smallest total volume achieving 80% conversion) other than the design proposed above? (10%)

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4. **(20%)** Silane, an inorganic compound with chemical formula SiH_4, is a practical precursor to Si and is widely applied in semiconductor factories. A 304 stainless cylinder with an internal volume of 50 liter is used to fill-up 15 kg of silane gas. Estimate the pressure in atm in this cylinder at room temperature using the following information. For SiH_4, critical temperature T_c = 269.70 K, critical pressure P_c = 47.77 atm, and acentric factor ω = 0.0938. Also answer the following questions.

(i) Pitzer correlation for the compressibility factor Z is $Z = Z^0 + \omega Z^1$, what are the functions of Z^0 and Z^1?

(ii) Pitzer correlated the compressibility factor Z with the second virial coefficient. Please start from $Z = 1 + \frac{BP}{RT}$ and $\hat{B} = B^0 + \omega B^1$ (where B is the second virial coefficient and $\hat{B}$ is its reduced form) to show Z^0 and Z^1 as functions of reduced pressure P_r and reduced temperature T_r.

(iii) B^0 and B^1 are adequately represented by the Abbott equations as

$$B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}, \qquad B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

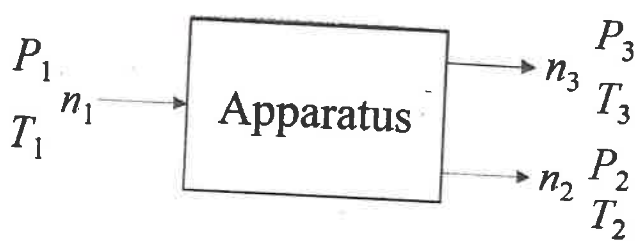
Using the above equations, calculate the compressibility factor of SiH_4 in the cylinder and then the vapor pressure inside. $R = 0.082$ liter·atm/(K·mol)

5. **(15%)** A thermodynamic steady-flow apparatus is designed to take a gaseous fluid at 20°C and 4 atm and separate it into two streams of equal molar flow rate, one at -20°C and 1 atm and the other at 1 atm and a hotter temperature, as shown in the diagram below. The apparatus operates adiabatically and no work required or produced. If the fluid can be esteemed as an ideal gas with a constant pressure heat capacity of $C_p^{ig} = 7/2\ R$, $R = 8.314\ J{\cdot}K^{-1}{\cdot}mol^{-1}$.

(i) Start from the first law of thermodynamics, $dU = dQ_{rev} - PdV$ and the definition equation of enthalpy, $H = U + PV$, to show the integration form of entropy change ΔS^{ig} from an initial state at temperature T_0 and pressure P_0 to a final state at T and P.

(ii) From the energy balance for this steady-state flow process, calculate the temperature of the hot stream if the flow rate of the input stream is 1 mol/s? The kinetic and potential energy terms can be omitted.

(iii) What is the entropy balance equation for this steady-state flow process? Also determine if this apparatus is thermodynamically feasible or not.



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6. **(15%)** Gold/Silicon (Au/Si) eutectic alloy system, characterized by a very low eutectic point of 363 ˚C, is a promising material for fabricating creating 3D structures and hermetic packaging in micro-electro-mechanical system (MEMS) devices. If the formation of single-phase alloy of Au_4Si can be thought as a substitutional solid solution where N is the total number of atom A (Au) and atom B (Si) (1N = Avogadro's number),

(i) calculate the number of atomic arrangements contained in this solid solution.

(ii) calculate the entropy change in J/(K·mol) for the formation of this solid solution.

Assume that change in lattice constant during the formation of solid-state solution is negligible. Stirling's approximation can be applied as $\ln N! = N\ln N - N$, when $N \gg 1$. Boltzmann constant (k_B) is 1.38×10^{-23} J·K^{-1}.

(iii) Consider an equiatomic alloy of CoCrFeMnNi in its solid solution state, i.e., the atomic ratio for each element is 0.2, calculate its configurational entropy increase of mixing per mole. Multicomponent alloys of this kind are also named as High-Entropy Alloys (HEAs) which show better strength-to-weight ratios. Please explain the reason of naming of HEAs.