1. (25 pts) Ethylene glycol (EG) is produced in a CSTR by the following reaction:

$$CH_2-CH_2\ (O) + H_2O \xrightarrow{H_2SO_4} CH_2-OH \mid CH_2-OH$$
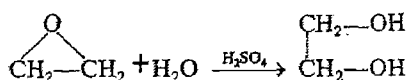
It is desired to produce 200 million pounds per year of EG. The CSTR reactor is operated isothermally. A 1 lb mol/ft^3 of ethylene oxide (EO) in water is fed to the reactor with an equal volumetric solution of water containing 0.9 wt % of the catalyst H$_2$SO$_4$. The specific reaction rate constant is 0.311 min^{-1}.

(a) (15 pts) If 80% conversion is to be achieved, determine the necessary reactor volume.

(b) (5 pts) If two 800-gal reactors are arranged in parallel. What is the corresponding conversion? (1 gal = 0.133 ft^3)

(c) (5 pts) If two 800-gal are arranged in series. What is the corresponding conversion?

2. (25 pts) NCU company is going to build a pilot plant to decompose pollutant A. The elementary reaction A → B + 2C is carried out isothermally in a flow reactor with no pressure drop. The reactant A enters the reactor at 5 atm and 127 °C and a molar flow rate of 2 mol/min.

(a) (15 pts) In order to determine the reaction parameters, a set of experiments were carried out in a constant-volume batch reactor. Runs 1 and 2 were carried out at 27 °C, while run 3 was carried out at 87 °C. From the data in the Table below, determine (1) the reaction order, (2) rate constant, and (3) activation energy. [R = 8.314 J/mol K]

Run	Initial Concentration, C_{Ao} (mol/L)	$-r_A$ (mol/L min)
1	0.025	2.5×10^{-6}
2	0.05	5.0×10^{-6}
3	0.05	0.0015

(b) (10 pts) Calculate the reactor volume of a PFR to achieve 90% conversion.

3. (25 pts) The solubility of a solid solute i in a compressed fluid at given temperature (T) and pressure (P) can be estimated via solving the equality of fugacity of solute i in its pure solid state (S) and in the fluid phase (F):

$$f_i^S(T,P) = \hat{f}_i^F\left(T, P, \underline{y}\right)$$

where $\underline{y}$ is the composition vector in term of mole fraction for the fluid. The solid phase fugacity of solute i can be determined through its sublimation pressure ($P_{\text{sub},i}$):

$$f_i^S(T, P) = P_{\text{sub},i} \cdot \exp\left[\frac{V_i^S(P - P_{\text{sub},i})}{RT}\right]$$

where V_i^S is the solid molar volume of solute i. The fugacity of solute i in the compressed fluid phase can be calculated from the fugacity coefficient of solute i ($\hat{\phi}_i$):

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$$\bar{f}_i^F\left(T, P, \underline{y}\right) = y_i P \bar{\phi}_i$$

Please estimate the solubility of anthracene ($C_{14}H_{10}$, abbreviation: ANT) in compressed ethylene (C_2H_4, abbreviation: ETH) at 25 °C and at total pressure of 10 bar using the above equations under following assumptions:

(a) **(12 pts)** Using the ideal-gas law to describe the fluid phase.

(b) **(13 pts)** Using the virial equation of state truncated after the second term to describe the fluid phase, i.e.,

$$\ln\bar{\phi}_i = \left(2\sum_{j=1}^{n} y_j B_{ij} - B_{\text{mixt}}\right)\frac{P}{RT}$$

where B_{mixt} is the second virial coefficient of the mixture. For the second virial coefficient B use the van der Waals result,

$$B_{ij} = b_{ij} - \frac{a_{ij}}{RT}$$

with $a_{ij} = \sqrt{a_i a_j}$ and $b_{ij} = 0.5(b_i + b_j)$. The van der Waals constants are related to the critical constants:

$$a_i = \frac{27 R^2 T_{c,i}^2}{64 P_{c,i}}$$

$$b_i = \frac{R T_{c,i}}{8 P_{c,i}}$$

Since the solubility of anthracene in compressed ethylene is very low, please assume $y_{\text{ANT}} \approx 0$, $y_{\text{ETH}} \approx 1$, and $B_{\text{mixt}} \approx B_{\text{ETH}}$ for determining fugacity coefficient of anthracene in fluid phase to avoid trial-and-error.
Properties of investigating compounds:

Compound	T_c (K)	P_c (MPa)	Density (g/cm³)	P_{sub} (Pa)
anthracene	877.75	3.39	1.28 (at 25 °C)	1.78×10^{-3} (at 25 °C)
ethylene	282.35	5.04	--	--

4. **(25 pts)** Cell membranes, arguably the most important boundary in nature, delineate cells and therefore define "life" in its most primordial form. While historically described as 2D homogeneous mixtures of lipids and proteins, cell membranes are now believed to be laterally heterogeneous and contain nano-sized domains known as *rafts*. Several theories have been proposed to explain the existence of rafts; one of them involves *liquid-liquid phase separation*, which is often explored by examining a three-component lipid membrane as a simplified model of cell membranes. In this model system, the membrane is homogenous when it is above the *critical temperature T_c*. Upon cooling below T_c, the membrane undergoes the liquid-liquid phase separation, where the initially homogeneous membrane transitions into the membrane possessing two stable coexisting phases, namely the *liquid-ordered (L_o)* and *liquid-disordered (L_d)* phases. (a) (2 pts) Give the conditions for which two phases can stably coexist at equilibrium. The L_o phase is considered as the physical manifestation of

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rafts, while L_d forms the matrix surrounding rafts. The phase separation can only occur for certain lipid compositions, as manifested in a compositional phase diagram mapped for such a three-component lipid membrane (see below). Only when the composition falls inside the dome-shaped region in the phase diagram can the membrane undergo phase separation upon cooling below T_c. One striking feature of the phase diagram is the presence of a *miscibility critical point*, marked by a star in the phase diagram. (b) (2 pts) How will the thermodynamic properties of L_o and L_d vary with respect to each other when the composition approaches the miscibility critical point from within the dome-shaped region? (c) (4 pts) Will the first derivative of Gibbs energy vary continuously or abruptly when a compositional change follows path A? What about the case for path B? Explain your answers.

To further explore the thermodynamics of raft formation, you decide to measure the entropy difference between L_o and L_d when they coexist. To this end, you envision an experiment on a lipid membrane with the composition marked by a diamond in the phase diagram. In this experiment, temperature of the membrane would be elevated, and the membrane phase is expected to transition from L_o to L_d via L_o-L_d coexistence at the phase-transition temperature T_t. You would determine T_t for the membrane under varied surface tension π, so that the data on T_t as a function of π can be acquired. To extract the entropy difference from the acquired data, you figure out that a 2D version of the *Clapeyron equation* is needed. (d) (3 pts) Given $dG = VdP - SdT$, where G is Gibbs energy, V is molar volume, P is pressure, and S is entropy, derive the Clapeyron equation. (e) (3 pts) By analogizing 2D surface with 3D space, derive a 2D version of the Clapeyron equation. With the $T_t - \pi$ data and the 2D Clapeyron equation available, you should be ready to determine the entropy difference between L_o and L_d. (f) (4 pts) Given that $T_t = 30°C$ for $\pi = 30$ mN/m, $T_t = 25°C$ for $\pi = 25$ mN/m and molecular areas of L_o and L_d are 50 Å^2 and 100 Å^2, respectively, determine the entropy difference between L_o and L_d when they coexist. (g) (3 pts) How would this entropy difference change if the membrane has a composition at the miscibility critical point? (h) (4 pts) Based on Gibbs phase rule, is this experiment a feasible way to determine the entropy difference between L_o and L_d? Explain your answer.

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