1. Production of ammonia (NH_3) takes place by the Haber-Bosch process. In this process, nitrogen reacts with hydrogen over a Fe catalyst to form ammonia. The reaction is shown below:

$$N_2 + 3H_2 \rightarrow 2NH_3$$

The standard enthalpy of formation of ammonia is -46.11 kJ/mol and its standard Gibbs free energy of formation is -16.45 kJ/mol at 298K.

a. Calculate the equilibrium constant of the reaction at 298K as written above. (7pts)
b. The reaction is sometimes written as $½N_2 + 3/2H_2 \rightarrow NH_3$. Quickly calculate the equilibrium constant for the reaction as written here. (4pts)
c. Write out the equilibrium condition for this reaction in terms of $y_{i=}$ and P. You may assume ideal gas (4pts)
d. What set of conditions would give you the highest equilibrium yield for ammonia? (3pts)
    a. High temperature, high pressure
    b. Low temperature, low pressure
    c. High temperature, low pressure
    d. Low temperature, high pressure
e. Why? (5 pts)
f. Why do you think that the industrial ammonia production process does not use the conditions you selected above? (4pts)
g. Assume that the enthalpy of the reaction is constant with temperature. Calculate the equilibrium constant at 773K (8pts)
h. A stream of 1 kmol/s of N_2 and 3 kmol/s of H_2 are fed into an isothermal reactor packed with Fe catalyst at 773K and 10 bar. Write out the mass balances for the three species in the reaction in terms of extent of reaction. (6 pts)
i. Write out the condition for equilibrium in terms of extent of reaction (4 pts)

2.

a. Estimate the saturation pressure of furfuryl alcohol at 303K. Its normal boiling point is 445K and its enthalpy of vaporization is 53.6 kJ/mol (6 pts)

b. What assumptions did you have to make? (4pts)

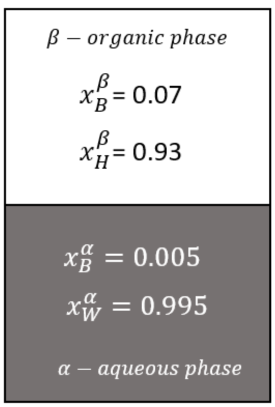
3. The reaction of acetic acid with butanol to produce butyl acetate processed to equilibrium at 308,15K. The reaction is shown below and it takes place in the liquid phase in an acetone solvent. The standard Gibbs free energies of formation and the activity coefficients for all reactive components in the system are shown in the table. All values are at the reaction temperature.

$$C_4H_{10}O + C_2H_4O_2 \rightarrow C_6H_{12}O_2 + H_2O$$

	1: butanol	2: acetic acid	3: butyl acetate	4: water
Δg^o_f (kJ/mol)	-146.0	-381.3	-306.5	-228.1
γ_l	1.9	2.2	1.2	6.0

a. Calculate the equilibrium constant of the reaction (7pts)
b. A liquid mixture of 1 mol butanol and 1 mol acetic acid 18 mol acetone (solvent) reacts to equilibrium. Write out mass balances for each of the four components in terms of extent of reaction (6pts)
c. Assuming that the solution is ideal, calculate the extent of reaction at equilibrium (6pts). You do not need to use an equation solver.
d. In reality, the mixture is not ideal. The activity coefficients of the compounds are shown in the table above. Calculate the extent of equilibrium (6pts) You do not need to use and equation solver.

4. Butanol is placed in a biological process, in which Clostridium acetobutylicum bacteria consume sugar and produce butanol. The butanol is extracted from the water by contacting the water stream with an organic solvent in a continuous extraction process at 308.15K. In one embodiment of this process, at the outlet of the extractor, the organic phase (phase β) has $x_b^\beta = 0.07$, while the aqueous phase (phase α) has $x_b^\alpha = 0.005$.



B: butanol
H: hexane
W: water

a. The 2-suffix Margules parameter for the butanol-hexane system is $A^{bh} = 4035$ J/mol. Calculate the activity coefficient of butanol in the organic (hexane) phase. (8pts)

b. Calculate the 2-suffix Margules parameter for the water butanol system. You may assume that the two streams exiting the extractor are in liquid-liquid equilibrium (12 pts)