

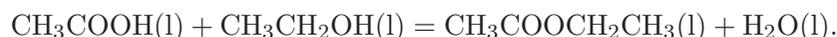
The heat capacities of the components are given by the equation

$$\frac{C_P}{R} = A + BT + CT^2 + \frac{D}{T^2},$$

with T in kelvin and with parameters given below:

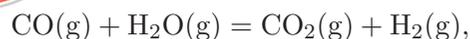
	A	$10^3 \times B$	$10^6 \times C$	$10^{-5} \times D$
SO ₂	5.699	0.801	–	–1.1015
O ₂	3.639	0.506	–	–0.227
N ₂	3.280	0.593	–	0.040
SO ₃	8.060	1.056	–	–2.028

Problem 14.18: Consider the esterification reaction



- Calculate the equilibrium constant at 25 °C.
- A reactor is loaded with a solution of acetic acid in ethanol containing 80% acetic acid by mole. The reaction is allowed to proceed to equilibrium at constant temperature of 25 °C. Assuming the components to form an ideal solution, calculate the composition of the equilibrium mixture.
- Repeat the calculation using activity coefficients calculated from UNIFAC.

Problem 14.19: ~~(40%)~~ The water gas shift reaction



is used to produce high-purity hydrogen. The reaction is carried out in a 10 m³ reactor that contains a copper catalyst and is operated at 1000 K and 1.5 bar. The equilibrium constant is given by

$$K(T) = e^{-5.057 + 4951.4/T},$$

where T is in K.

- Is the reaction exothermic or endothermic?
- Calculate the value of K_P at 1000 K, with P in bar. What are the units of K_P ?
- The composition of the reactor feed is 1 mole of CO and 5 moles of steam. Assuming the reaction to reach equilibrium, what is the composition (in terms of mole fraction) of the stream exiting the reactor?
- After reading your report, your boss points out that for fuel cell applications, the mol fraction of CO must not exceed 5×10^{-3} in order to avoid poisoning of