Problem 1 (50 points)

Water and ethanol are known to form an azeotrope. However, simplified thermodynamic models that assume ideal mixtures cannot predict the formation of the azeotrope. Let the total pressure P be 101.325 kPa.

(a) *(15 points)* Use your preferred software package (e.g., MATLAB, MS Excel etc.) and the given data for (1) water molar fraction, x_1, and temperature, T (^oC) (see file `Water_Temp_Data.txt`), to plot an x-y diagram for (2) ethanol. Assume an ideal mixture.

(b) *(30 points)* Use Aspen Plus with a suitable thermodynamic model to obtain an x-y diagram for (2) ethanol. Vary the water mole fraction, and choose 51 points for its range of values. Indicate the azeotrope location in the plot.

(c) *(5 points)* What type of azeotrope is formed?

Solution

(a) A spreadsheet in MS Excel is shown in Figure 1.1. Raoult's Law was used in which the saturation pressures were calculated with the Antoine equation. The coefficients were taken from Table B.2 in Smith, van Ness, & Abbott's book (7th Edition). Note that this ideal model does not capture the azeotrope.

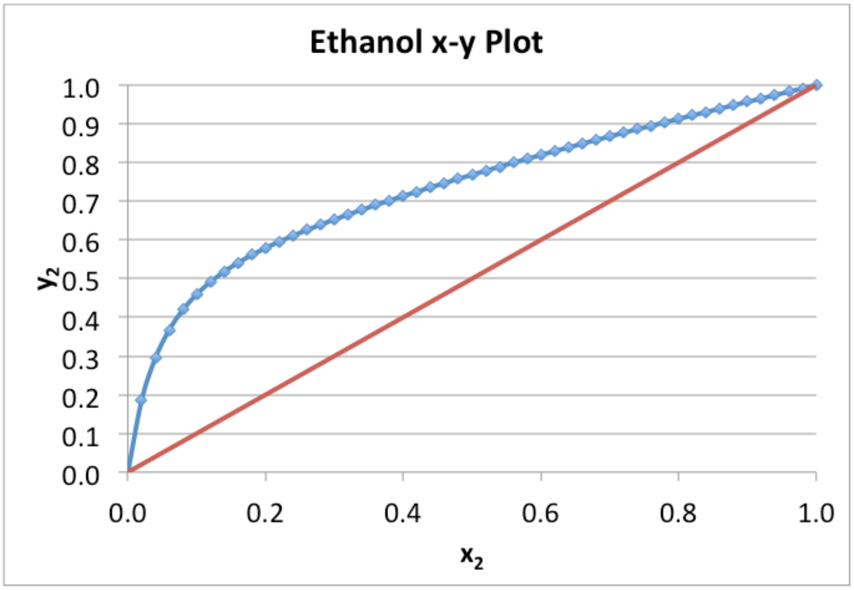

Figure 1.1 x-y plot for ethanol using Raoult's Law (ideal solution model).

(b) The plot obtained in Aspen Plus is shown in Figure 1.2. The thermodynamic model chosen was NRTL.

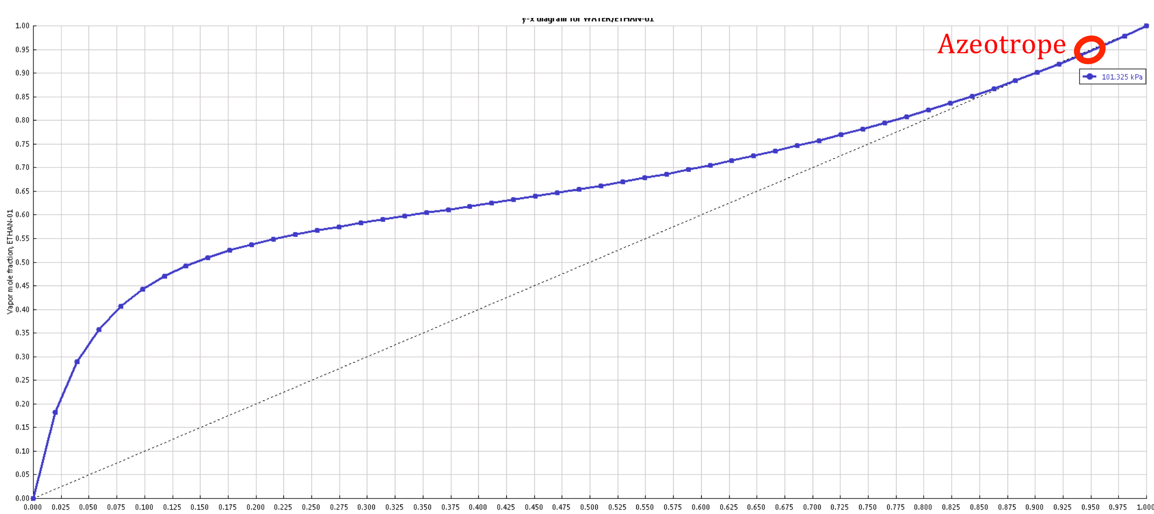

Figure 1.2 x-y plot for ethanol using Aspen Plus (NRTL model).

(c) Water and ethanol form a positive (or minimum-boiling) azeotrope, since the azeotrope boils at a lower temperature than its constituents as can be seen in a T-x-y plot (Figure 1.3).

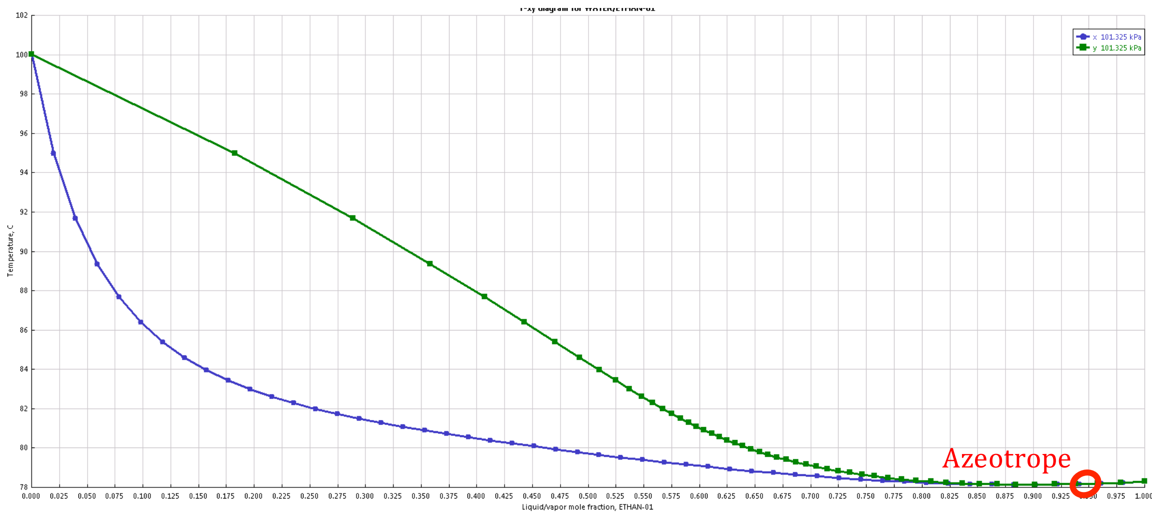

Figure 1.3 T-x-y plot for water and ethanol using Aspen Plus (NRTL model).

Problem 2 (50 points)

Styrene (C_8H_8) and hydrogen (H_2) are produced from ethylbenzene (C_8H_{10}) by catalytic dehydrogenation. Styrene production from ethylbenzene requires a large amount of steam (water), both to heat the reactor and to prevent coking; coking is the reaction that produces coke, a C_xH_y polymer (where often, $x \approx y$).

The reactor outlet stream is cooled in a separator, creating three phases: a water phase, an organic phase, and a vapor phase (see Figure 2.1). The water phase is practically 100% water; the vapor phase is mostly hydrogen; and the organic phase contains predominant amounts of unreacted ethylbenzene and styrene product. Perform a flash calculation in Aspen Plus and show the stream table of results.

Given:

- Reactor outlet stream
  - 35 kmol/h of unreacted ethylbenzene;
  - 65 kmol/h of styrene;
  - 65 kmol/h of hydrogen;
  - 3000 kmol/h of steam;
  - $T = 620$ °C and $P = 1$ atm.
- 3-phase flash
  - $T = 25$ °C and $P = 1$ atm.

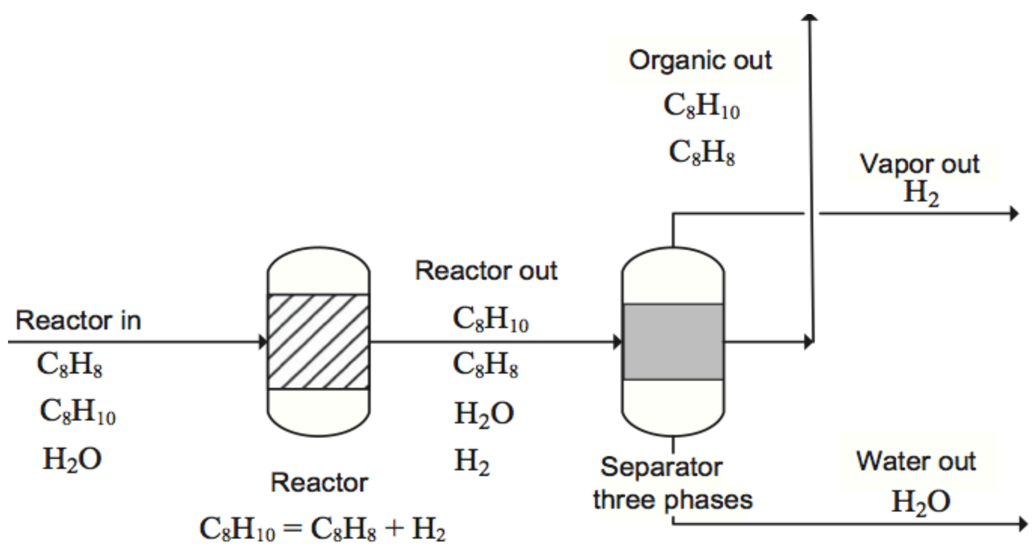

Figure 2.1 Styrene production flowsheet.

Solution

The thermodynamic model chosen was PENG-ROB. Figure 2.2 shows the flowsheet in Aspen Plus. Table 2.1 shows the stream table of results.

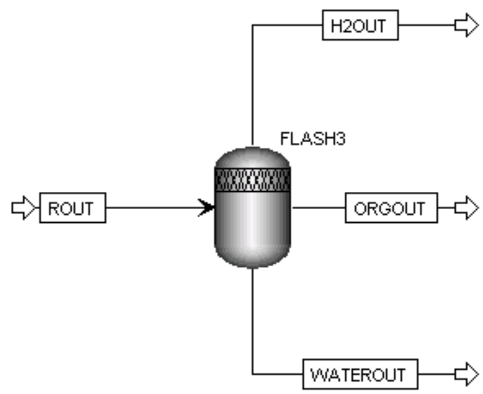

Figure 2.2 3-phase flash block in Aspen Plus.

Table 2.1 Stream table of results for the 3-phase flash separator system.

	Units	H2OUT	ORGOUT	ROUT	WATEROUT
From		FLASH3	FLASH3		FLASH3
To				FLASH3	
Substream: MIXED					
Phase:		Vapor	Liquid	Vapor	Liquid
Component Mole Flow					
ETHYL-01	KMOL/HR	0.31	34.69	35.00	0.00
STYRE-01	KMOL/HR	0.39	64.61	65.00	0.00
HYDRO-01	KMOL/HR	64.97	0.03	65.00	0.00
WATER	KMOL/HR	1.73	3.88	3000.00	2994.40
Component Mole Fraction					
ETHYL-01		0.00	0.34	0.01	0.00
STYRE-01		0.01	0.63	0.02	0.00
HYDRO-01		0.96	0.00	0.02	0.00
WATER		0.03	0.04	0.95	1.00
Mole Flow	KMOL/HR	67.40	103.20	3165.00	2994.40

Mass Flow	KG/HR	235.77	10481.93	64662.58	53944.88
Volume Flow	CUM/HR	1649.58	11.78	231836.00	54.27
Temperature	C	25.00	25.00	620.00	25.00
Pressure	BAR	1.01	1.01	1.01	1.01
Vapor Fraction		1.00	0.00	1.00	0.00
Liquid Fraction		0.00	1.00	0.00	1.00
Solid Fraction		0.00	0.00	0.00	0.00
Molar Enthalpy	KCAL/MOL	-1.25	12.38	-47.99	-68.73
Mass Enthalpy	KCAL/KG	-356.06	121.85	-2348.82	-3814.86
Enthalpy Flow	GCAL/HR	-0.08	1.28	-151.88	-205.79
Molar Entropy	CAL/MOL-K	-0.59	-83.81	-0.80	-40.12
Mass Entropy	CAL/GM-K	-0.17	-0.83	-0.04	-2.23
Molar Density	MOL/CC	0.00	0.01	0.00	0.06
Mass Density	KG/CUM	0.14	889.65	0.28	993.96
Average Molecular Weight		3.50	101.56	20.43	18.02

Problem 3 (50 points)

Consider an ammonia plant with a feed stream containing 100 lbmol/h of nitrogen and 300 lbmol/h hydrogen (with no impurities) as shown in Figure 3.1. This feed is catalytically reacted to produce ammonia. The reactor operates at high pressure (≈ 2000 psia). The equilibrium reaction is $N_2 + 3\ H_2 = 2\ NH_3$. Reaction products are refrigerated and separated to −28 °F in a general equilibrium flash. Use Aspen Plus to compute the molar flowrate of ammonia in the liquid phase out of the flash unit.

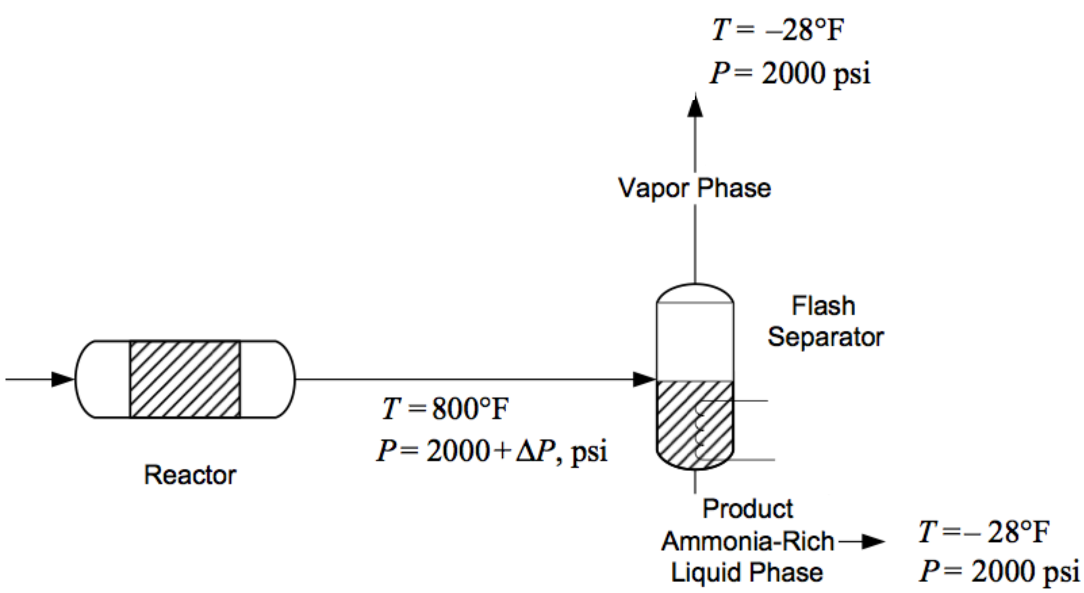

Figure 3.1 Ammonia synthesis reactor-flash flowsheet.

Solution

The thermodynamic model chosen was SRK. Figure 3.2 shows the flowsheet in Aspen Plus. The molar flowrate of ammonia in the NH3RICH stream is 77.63 lbmol/h.

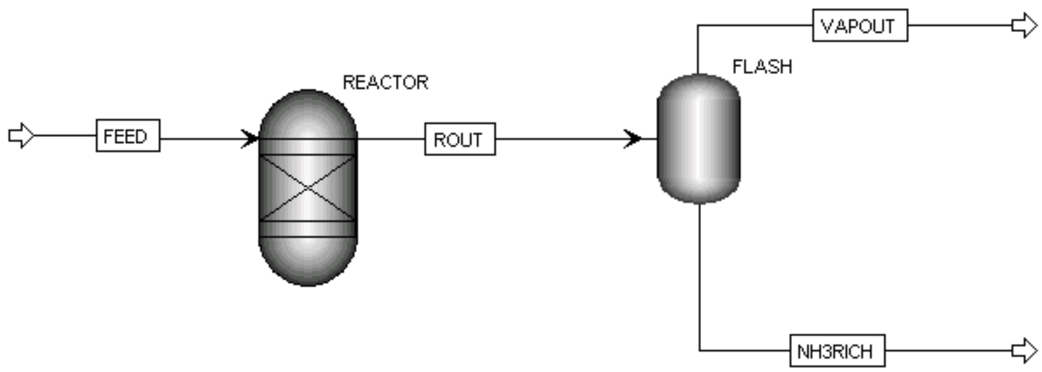

Figure 3.2 Ammonia synthesis flowsheet in Aspen Plus.