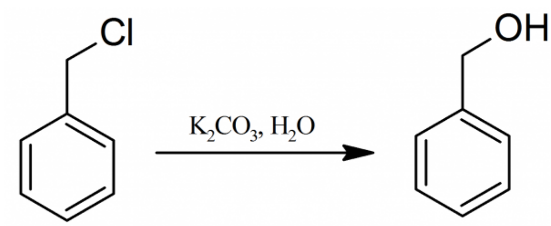
Chemical Engineering Thermodynamics
Quiz 4 February 4, 2021

Benzyl alcohol (BnOH) has a high index of refraction close to that of silica, cotton and wool so that if a cotton ball or fumed silica powder are immersed in BnOH they become almost invisible. It is also used as an antiseptic and as a flavor enhancing food additive as well as use as a treatment for head lice strangely enough. BnOH is made from toluene (which is a direct fraction from petroleum refining) via BnCl. BnCl is boiled in water in the presence of potassium carbonate (10%) under reflux. The reaction is run to 30% conversion to avoid chlorination of the aromatic group. BnOH is purified by flash distillation from a fraction at 474 K.

	T_b, K	ΔH_v, kJ/mole	$\Delta_f H_0$ (l), kJ/mole	C_p (l), J/(mole K)
BnCl (l)	335	48.6	-33	A = 182; B = C = D = 0
BnOH (l)	478	63	-164	A = 218; B= C = D = 0
K_2CO_3 (l)			-1,130	A = 209; B = -1.63e-7; C = 8.01e-8; D = -1.34e-8
Water (l)	373	40.7	-285	A = 72.4; B = 0.0104; C = -1.49e-6; D = 0
HCl (g)			-92.3	A = 30.7; B = -0.0072; C = 1.25e-5; D = -3.90e-9



a) Write a balanced reaction for this synthesis.
b) Make a table of the moles feeding into the reactor and the moles flowing out of the reactor for each of the five species ***using as a basis a total of one mole for the feed stream***. The reaction feed is 62 mole percent water/K_2CO_3 mixture with a 90/10 molar ratio. The reaction is run to 30% completion.
c) Use the heat of formation method for the energy balance to **determine the heating or cooling** that is required for this reaction per mole of the feed stream. The feed temperature is 298 K, the reaction temperature is 374 K. Assume the reactor is adiabatic. Is the reaction **endothermic or exothermic** under these conditions?
d) The products are separated in a flash tank from a mixture of water, BnOH, BnCl at 201°C (474 K)) by distillation. The feed stream is liquid with 54 mole % water, 14 mole % BnOH, and 32 mole % BnCl **at 320 K**. The liquid stream exiting the flash distillation, **B**, is 99% BnOH; the vapor stream, **V**, is 1 % BnOH and both streams are at 474 K. **Make a table of the mole fractions and moles of the three components in the three streams of the flash tank.** Assume that the ratio of BnCl to water in streams **B** and **V** is the same as in stream **F**. ***Use as a basis one mole for the sum of the components in F.***
e) **Find the heat load** for the separation (kJ/mole of the feed stream, **F**). Is this an **endothermic or exothermic** process?

ANSWER SHEET:

For the answers please fill out the following answer sheet below and send a pdf of the excel sheet printed in landscape.

a) Balance Equation:

b) Table **in Excel Sheet** pdf.

c) Heating or Cooling Required:

Endo or exothermic?

d) Table in **Excel Sheet** pdf.

e) Heat Load:

Endo or exothermic?

You can **use the attached excel sheet** to do your calculations. Please **write down all equations** that you use in the Excel sheet on your work sheet and turn it in with the quiz.

(a) $C_7H_7Cl + H_2O \rightleftharpoons C_7H_8O + HCl$

(b) $X_{water/K_2CO_3} = 0.62$

Feed

$X^F_{BnCl} = 0.38$

$X^F_{water} = 0.9(0.62) = 0.558$

$X^F_{K_2CO_3} = 0.1(0.62) = 0.062$

$n^F_{BnOH} = 0$

$n^F_{HCl} = 0$

$n^F_{BnCl} = 1\,mole\ 0.38 = 0.38\,moles$

$n^F_{water} = 0.558\,moles$

$n^F_{K_2CO_3} = 0.062\,moles$

Conversion of BnCl is 30%

$n^{Product}_{BnCl} = 0.38\,moles \cdot 0.70 = 0.266\,moles$

change is $0.38\,mol - 0.266\,mol = 0.114\,moles$

$n^{Product}_{BnOH} = 0.114\,moles$

$n^P_{HCl} = 0.114\,moles$

$n^P_{K_2CO_3} = 0.062\,moles$ unchanged

$n^P_{water} = 0.558\,moles - 0.114\,mol = 0.444\,moles$

(c)

Feed is at 298K so $\int_{298}^{298} C_p\,dT = 0$

Feed Enthalpy is $\sum_i (\Delta H^0_f)_{i,298K}\, n^F_i$ for reactants

Product Enthalpy is $\sum \left(\Delta H^0_f\, n^P_i + n_i \int_{298K}^{379K} C_p\,dT \right)$

Total = Product − Feed = 16.4 KJ/one mole Feed — Endothermic

(d)

$F = V + B = 1\,mole$

$V = 1\,mole - B$

$n^{F}_{BnCH} = 0.14\,moles = 0.99\,B + 0.01\,V\,(1\,mole - B)$

$B = \frac{0.14\,moles - 0.01\,mole}{0.99 - 0.01}$

$= 0.133\,mole$

$V = 1\,mole - 0.134\,mole = 0.867\,mole$

For the BnCl/water fraction of F

$x^{F}_{BnCl\ in\ BnCl/water} = \frac{0.32\,moles}{0.32 + 0.59\,moles} = 0.372$

$x^{F}_{water\ in\ BnCl/water} = 0.628$

$x^{V}_{BnCl} = 0.372(1 - 0.01) = 0.368$

$x^{B}_{BnCl} = 0.372(1 - 0.99) = 0.004$

$x^{V}_{H_2O} = 0.628(0.99) = 0.622$

$x^{B}_{H_2O} = 0.628(0.01) = 0.006$

(e) Use as a reference state F @ 320K so $H^F = 0$ kJ/mole F

$H^V = \sum_i n_i \left(\int_{320K}^{T_b} Cp_i\,dT + \Delta H^{T_b}_{v,i} + \int_{T_b}^{434K} Cp_i\,dT \right)$

$H^B = \sum_i n_i \left(\int_{320K}^{434K} Cp_i\,dT \right)$ Total $= H^V + H^B = 58.1$ kJ/mole F

Endothermic

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Calculate Cp Integrals

Material	Ti, K	Tf, K	A	B	C	D	Cp integral, J/mole (J/mole)	DH formation (kJ/mole)	T boiling, K (K)	DH Vaporization (kJ/mole)	Moles in	Moles out	Moles in * Cp integral (298->Tin) (Joules)	Moles Out * Cp integral (298->Tout) (Joules)	Moles in * DfH0 (kJ)	Moles out * DfH0 (kJ)	Material
BnCl (l)	298	374	182	0	0	0	13832	-33	335	49	0.38	0.266	0	3679	-12.5	-8.8	BnCl
BnOH (l)	298	374	218	0	0	0	16568	-164	478	63	0	0.114	0	1889	0.0	-18.7	BnOH
K2O3 (l)	298	374	209	-1.63E-07	8.01E-08	-1.34E-08	15846	-1130			0.062	0.062	0	982	-70.1	-70.1	K2O3
H2O (l)	298	374	72.4	0.0104	-1.49E-06	0.00E+00	5755	-285	373	40.7	0.558	0.444	0	2555	-159.0	-126.5	H2O
HCl (g)	298	374	30.7	-0.0072	1.25E-05	-3.90E-09	2246	-92.3			0	0.114	0	256	0.0	-10.5	HCl
												Sums:	0	9362	-242	-235	

Q load — Heat of Formation per mole feed

Qbar	
16.4	kJ

Separation

	Temp,	Moles	xBNOH	xBNCl	xWater	moles nBNOH	moles nBNCl	moles nWater	
L, Feed	320	1	0.14	0.32	0.54	0.140	0.320	0.540	L, Feed
V	474	0.867	0.01	0.368	0.622	0.009	0.319	0.539	V
B	474	0.133	0.99	0.004	0.006	0.132	0.001	0.001	B

You need to type in equations and values to do the proper calculations in the green boxes

kJ — Vapor Stream (V)

	L320->LTb	LTb->VTb	VTb->V474	Sum*moles
BNOH	34.4	63.0	-0.9	0.8
BNCl	2.7	49.0	25.3	24.6
Water	4.0	40.7	7.7	28.3
			Sum	53.7

	Tb, K	DHv, kJ/mole
BNOH	478	63
BNCl	335	49
Water	373	40.7

kJ — B Stream (L)

	L320->L474	Value * moles
BNOH	33.6	4.42
BNCl	28.0	0.01
Water	11.7	0.01
	Sum	4.45

Take Liquid at 320K as the reference state

Q/mole of L	58.1	kJ/mole L feed