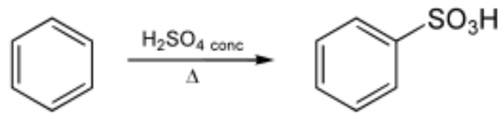
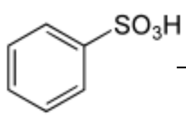
Quiz 4
Chemical Engineering Thermodynamics
February 2, 2017

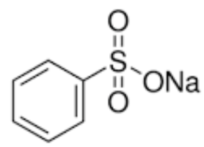
Sodium benzene sulfonate is a common hydrotrope used in detergent formulations. It is produced by the following two reactions at Nease Performance Chemicals in Harrison:



$+ H_20$ I



$+$ NaOH =>



$+ H_20$ II

		KJ/mole	J/(mol K)	g/mole
State	Compound	DHf298 (L)	Cp (L)	Mol. Wt.
Liquid	Benzene	49.1	136	78
Liquid	H2SO4	-814	139	98
Liquid	Benz. Sulf. Acid	11.5	150	158
Liquid	Water	-286	75.3	18
Liquid	NaOH	-426	59.5	40
Liquid	Sodium Benz. Sulf.	11.5	150	181
Solid	Na2SO4	-1390	157	142
Gas Constant		8.314	g/(mol K°)	

a) Reaction I is carried out in a batch reactor with the reactants initially at 30°C. The reaction is terminated at 50% conversion of benzene and the reactor is 50°C when the reaction is terminated. On the basis of 1 mole of benzene and 2 moles of H_2SO_4 feed what heating or cooling is required? Is this an endothermic or exothermic reaction? (Include the water in the concentrated sulfuric acid in the feed stream. Concentrated sulfuric acid is 98% by weight (92 molar %) sulfuric acid in water).
Make a table of v, n_{in}, n_{out}, ΔH_f, C_p for this reaction, then do the calculation.

b) Reaction I is terminated by neutralization of H_2SO_4 with NaOH (caustic), 50 wt. % (31 mole %) in water. Based on 1 mole of H_2SO_4 and 1.333 moles of NaOH, a starting temp. of 50°C and an end temp. of 80°C, do you cool or heat and what heating or cooling is required? Endothermic or exothermic reaction? Use 100% conversion (neutralization).
NaOH (aq) + H_2SO_4 (l) => H_2O + Na_2SO_4 (s)
(Solids fall out of solution by precipitation. Include residual water from Reaction I and the products and residual reactants from Reaction I based on 1 mole H_2SO_4.)
Make a table of v, n_{in}, n_{out}, ΔH_f, C_p for this reaction, then do the calculation.

c) Determine the cooling or heating necessary for reaction II using one mole of benzyl sulfonic acid as a basis with 100% conversion. The starting temperature is 80°C and the end temperature 90°C. Include the residual materials from (a) and (b) except for the Na_2SO_4 solid.
Just Make a table of v, n_{in}, n_{out}, ΔH_f, C_p for part "(c)", **do not do the calculations**.

Answers Quiz 4
ChE Thermodynamics

a)

	ν	mole n_{in}	mole n_{out}	kJ/mole $H_{f\,298K}$	kJ/mole C_{pL}
Benzene	-1	1	0.5	49.1	0.136
H_2SO_4	-1	2	1.5	-814	0.139
Water	1	0.16	0.66	-286	0.0753
BSA	1	0	0.5	11.5	0.150

$$\Delta T_{in} = 5\,K^\circ \quad \Delta T_{out} = 25\,K^\circ$$

$$\Sigma H_{in} = \Sigma n_{in}\left(H_{f_{298}} + C_p \Delta T\right)$$

$$= 1\,\text{mole}\left(49.1\tfrac{kJ}{mol} + 0.136\tfrac{kJ}{mol\,K^\circ}\,5\,K^\circ\right)$$

$$+ 2\,\text{mole}\left(-814\tfrac{kJ}{mol} + 0.139\tfrac{kJ}{mol\,K^\circ}\,5\,K^\circ\right)$$

$$+ 0.16\,\text{mole}\left(-286\tfrac{kJ}{mol} + 0.0753\tfrac{kJ}{mol\,K^\circ}\,5\,K^\circ\right)$$

$$= 49.8\tfrac{kJ}{} + \left(-1{,}630\tfrac{kJ}{}\right) + \left(-45.7\tfrac{kJ}{}\right)$$

$$= -1{,}620\ kJ$$

$$\Sigma H_{out} = \Sigma n_{out}\left(H_{f_{298}} + C_p \Delta T\right)$$

$$= 0.5\,\text{mole}\left(49.1\tfrac{kJ}{mol} + 0.136\tfrac{kJ}{mol\,K^\circ}\,25\,K^\circ\right)$$

$$+ 1.5\,\text{mole}\left(-814\tfrac{kJ}{mol} + 0.139\tfrac{kJ}{mol\,K^\circ}\,25\,K^\circ\right)$$

$$+ 0.66\,\text{mole}\left(-286\tfrac{kJ}{mol} + 0.0753\tfrac{kJ}{mol\,K^\circ}\,25\,K^\circ\right)$$

$$+ 0.5\,\text{mole}\left(11.5\tfrac{kJ}{mol} + 0.150\tfrac{kJ}{mol\,K^\circ}\,25\,K^\circ\right)$$

$$= 26.3\,kJ + (-1{,}220\,kJ) + (-188\,kJ) + (7.63\,kJ)$$

$$= -1{,}370\ kJ$$

$\Delta H = \Sigma H_{out} - \Sigma H_{in}$

$= -1370\ kJ - (-1{,}620\ kJ)$

$= +250\ kJ$ Endothermic so heat is required

b)

	ν	mole n_i	mole n_o	kJ/mole $\Delta H_{f,298}$	kJ/mol K C_p
NaOH	-1	1.333	0.333	-426	0.0595
H_2SO_4	-1	1	0	-814	0.139
H_2O	1	0.44	1.44	-286	0.0753
Na_2SO_4	1	0	1	-1390	0.157
ϕ	0	0.333	0.333	49.1	0.136
BSA	0	0.333	0.333	11.5	0.150

$\Delta T_{in} = 25\ K^\circ$ $\Delta T_{out} = 55\ K^\circ$

$\Sigma H_{in} = \Sigma n_i (H_{f_{298}} + C_p \Delta T)$

$= 1.33\ mole \left(-426 \frac{kJ}{mol} + 0.0595 \frac{kJ}{mol\,K^\circ}(25\ K^\circ)\right)$

$+ 1.44\ mol \left(-286 \frac{kJ}{mol} + 0.0753 \frac{kJ}{mol\,K^\circ}(25\ K^\circ)\right)$

$+ 1\ mole \left(-1390 \frac{kJ}{mol} + 0.157 \frac{kJ}{mol\,K^\circ}(25\ K^\circ)\right)$

$+ 0.333\ mol \left(49.1 \frac{kJ}{mol} + 0.136 \frac{kJ}{mol\,K^\circ}(25\ K^\circ)\right)$

$+ 0.333\ mol \left(11.5 \frac{kJ}{mol} + 0.150 \frac{kJ}{mol\,K^\circ}(25\ K^\circ)\right)$

$= -565\ kJ + (-409\ kJ) + (-1386\ kJ) + 17.5\ kJ + 5.08$

$= -1210\ kJ$

$$\Sigma H_{out} = \Sigma n_o (H_{f_{298}} + C_p \Delta T)$$

$$= 0.333 \text{ mole} \left(-426 \tfrac{kJ}{mol} + 0.0595 \tfrac{kJ}{mol\,°K} (55\,K°)\right)$$

$$+ 1.44 \text{ mole} \left(-814 \tfrac{kJ}{mol} + 0.139 \tfrac{kJ}{mol\,°K} (55\,°K)\right)$$

$$+ 1 \text{ mole} \left(-1390 \tfrac{kJ}{mole} + 0.157 \tfrac{kJ}{mol\,°K} (55\,°K)\right)$$

$$+ 0.333 \text{ mole} \left(49.1 \tfrac{kJ}{mole} + 0.136 \tfrac{kJ}{mol\,°K} (55\,°K)\right)$$

$$+ 0.333 \text{ mole} \left(11.5 \tfrac{kJ}{mol} + 0.150 \tfrac{kJ}{mol\,°K} (55\,°K)\right)$$

$$= -141\,kJ + (-1160) + (-1380\,kJ) + 18.8\,kJ + 6.58\,kJ$$

$$= -2{,}660\,kJ$$

$$\Delta H = \Sigma H_{out} - \Sigma H_{in}$$

$$= -2660^{kJ} - (-1210^{kJ})$$

$$= -1{,}450\,kJ$$

Exothermic
Release Heat

c)

	ν	mol n_i	mole n_o	kJ/mole $\Delta H_{f,298}$	kJ/(mol K°) C_p
BSA	-1	1	0	11.5	0.150
NaOH	-1	1	0	-426	0.0595
NaBSA	1	0	1	11.5	0.150
H_2O	1	4.32	5.32	-286	0.0753
ф	0	1	1	49.1	0.136

$\Delta T_{in} = 55K°$ $\Delta T_{out} = 65K°$

Calculating <u>Net</u> part of the answer.

$$\Sigma H_{in} = \Sigma n_i (H_{f,298} + C_p \Delta T)$$

$$1 \text{ mol} \left(11.5 \tfrac{kJ}{mole} + 0.150 \tfrac{kJ}{mol\,K°} (55 K°)\right)$$

$$+ 1 \text{ mol} \left(-426 \tfrac{kJ}{mol} + 0.0595 \tfrac{kJ}{mol\,K°} (55 K°)\right)$$

$$+ 4.32 \text{ mol} \left(-286 \tfrac{kJ}{mol} + 0.0753 \tfrac{kJ}{mol\,K°} (55 K°)\right)$$

$$+ 1 \text{ mol} \left(49.1 \tfrac{kJ}{mol} + 0.136 \tfrac{kJ}{mol\,K°} (55 K°)\right)$$

$$= 19.8 \text{ kJ} + (-423 \text{ kJ}) + (-1220 \text{ kJ}) + 56.6 \text{ kJ}$$

$$= -1,570 \text{ kJ}$$

$$\Sigma H_{out} = \Sigma n_{out} (H_{f_{25C}} + C_{p_i} (65K^\circ))$$

$$= 1\,mole \left(11.5 \frac{kJ}{mole} + 0.150 \frac{kJ}{mol\,K^\circ}(65K^\circ)\right)$$

$$+ 5.32\,mole \left(-286 \frac{kJ}{mol} + 0.0753 \frac{kJ}{mol\,K^\circ}(65K^\circ)\right)$$

$$+ 1\,mole \left(49.1 \frac{kJ}{mol} + 0.136 \frac{kJ}{mol\,K^\circ}(65K^\circ)\right)$$

$$= 21.3\,kJ + (-1500\,kJ) + 57.9\,kJ$$

$$= -1421\,kJ$$

$$\Delta H = -1421\,kJ - (-1370\,kJ)$$

$$= -51\,kJ$$

This reaction is ~~endo~~ exothermic
but almost energy neutral
it generates heat