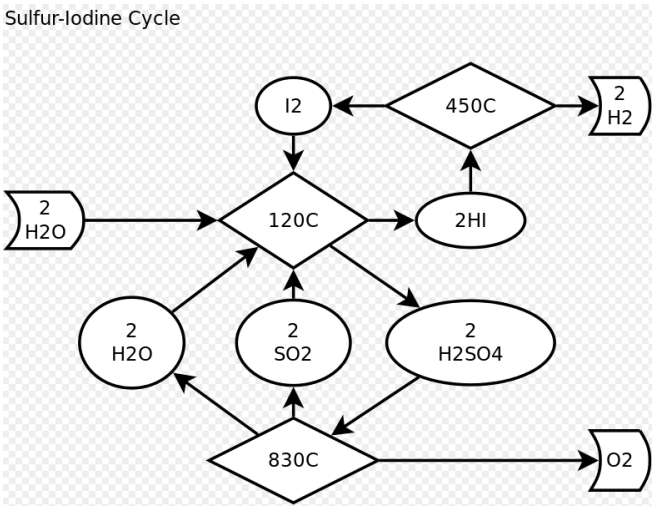
Quiz 13
Chemical Engineering Thermodynamics
April 23, 2020

The sulfur-iodine cycle has been proposed to produce hydrogen from water using concentrated solar energy in a continuous process that consumes only water and produces only hydrogen and oxygen. The process uses three simple reactions. *Assume that all of the reactants are in the gas phase*.



At the bottom of the diagram above, H_2SO_4 decomposes into H_2O, oxygen and sulfur dioxide. The reaction is:

$$2\ H_2SO_4\ (g) \Leftrightarrow O_2\ (g)\ + 2\ SO_2\ (g)\ + 2\ H_2O\ (g) \qquad \text{Reaction (1)}$$

Consider that you will initially react ***two moles of H_2SO_4*** and that there are initially ***no other reactants present***. Use a pressure of ***1 bar***. Turn in the next page with a filled out table containing your answers.

a) It is desired to determine the minimum temperature for this reaction to produce 99 percent conversion of the feed H_2SO_4. Use the attached Kcalc.xls spreadsheet and the data in the spreadsheet. (*In you answer included a detailed description of what you put into the spreadsheet and all of your work. Take a screen shot of the spread sheet and include that and your calculations/description with your answer.*)
b) What temperatures would be required to for 99.9 percent conversion? (*In you answer included a detailed description of what you put into the spreadsheet and all of your work. Take a screen shot of the spread sheet and include that and your calculations/description with your answer.*)
c) Using the temperature indicated in the diagram above, 830°C, what conversion is possible? (*In you answer included a detailed description of what you put into the spreadsheet and all of your work. Take a screen shot of the spread sheet and include that and your calculations/description with your answer.*)

d) What pressure would be required to obtain exactly 99 percent conversion at 800 K? (*In you answer included a detailed description of what you put into the spreadsheet and all of your work. Take a screen shot of the spread sheet and include that and your calculations/description with your answer.*)

e) At the bottom of the Kcalc.xls spreadsheet data is given for the Gibbs energy of formation at 800K for the reactants in Reaction (1). Use these values to do a Gibbs minimization at 800K and with P = 1 bar in order to determine the reaction coordinate using the same concentration of reactants as in part (a). **This is similar to example 17.12.** (*In you answer included a detailed description of what you put into the spreadsheet and all of your work. Take a screen shot of the spread sheet and include that and your calculations/description with your answer.*)

	Conversion of H2SO4	**T, K**	**P, bar**
a)	0.99		1
b)	0.999		1
c)			1
d)	0.99		
e)		800	1

Your Name:_____

Answers

	Conversion of H2SO4	T, K	P, bar
a)	0.99	869 (596°C)	1
b)	0.999	951 (678°C)	1
c)	1	1103 (830°C)	1
d)	0.99	800	0.209
e)	0.909	800	1

a) **869K** (596°C) b) **951K** (678°C)

Kcalc Sheet for Quiz 13 2020

Stoichiometric Number	Name	$\Delta H^\circ_{f,298}$ (kJ/mol)	$\Delta G^\circ_{f,298}$ (kJ/mol)	Constants for C_P in J/mol-K a	b	c	d
-2	H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08
1	O2	0	0	28.11	-3.70E-06	1.75E-05	-1.07E-08
2	SO2	-296.8	-300.14	23.85	6.699E-02	-4.610E-05	1.328E-08
2	H2O	-242	-229	32.24	1.924E-03	1.055E-05	3.596E-09
0	I2 (g)	62.42	-15.27	37.79	2.214E-04	-9.126E-07	1.035E-09
0	HI	26.5	-34.9	29.05	4.690E-03	4.912E-06	-2.654E-09
0	H2	0	0	27.14	9.274E-03	-1.381E-05	7.645E-09

enter all species above line 14

Reaction T(K)	869.286735	P, bar
ΔH°_T (kJ/mol)	390.569	1
ΔG°_T (kJ/mol)	-41.459	
ln K_a	5.736123738	
K_a	309.8609778	

Intermediate Calculations, J and I defined in text

Δa	Δb	Δc	Δd
45.7116	-2.428E-01	2.426E-04	-6.463E-08

R (kJ/mol-K)	0.0083145
ΔH°_{298} (kJ/mol)	403.536
ΔG°_{298} (kJ/mol)	248.658
ln $K_{a,298}$	-100.30739
J (kJ/mol)	398.68458
I	-33.134308

Rxn 1	
Rxn Coord	Test
0.99	-6.34626E-05

Kcalc Sheet for Quiz 13 2020

Stoichiometric Number	Name	$\Delta H^\circ_{f,298}$ (kJ/mol)	$\Delta G^\circ_{f,298}$ (kJ/mol)	Constants for C_P in J/mol-K a	b	c	d
-2	H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08
1	O2	0	0	28.11	-3.70E-06	1.75E-05	-1.07E-08
2	SO2	-296.8	-300.14	23.85	6.699E-02	-4.610E-05	1.328E-08
2	H2O	-242	-229	32.24	1.924E-03	1.055E-05	3.596E-09
0	I2 (g)	62.42	-15.27	37.79	2.214E-04	-9.126E-07	1.035E-09
0	HI	26.5	-34.9	29.05	4.690E-03	4.912E-06	-2.654E-09
0	H2	0	0	27.14	9.274E-03	-1.381E-05	7.645E-09

enter all species above line 14

Reaction T(K)	951.0409964	P, bar
ΔH°_T (kJ/mol)	388.687	1
ΔG°_T (kJ/mol)	-82.002	
ln K_a	10.37028625	
K_a	31897.60622	

Intermediate Calculations, J and I defined in text

Δa	Δb	Δc	Δd
45.7116	-2.428E-01	2.426E-04	-6.463E-08

R (kJ/mol-K)	0.0083145
ΔH°_{298} (kJ/mol)	403.536
ΔG°_{298} (kJ/mol)	248.658
ln $K_{a,298}$	-100.30739
J (kJ/mol)	398.68458
I	-33.134308

Rxn 1	
Rxn Coord	Test
0.999	0.094875839

c) **100% conversion**

Kcalc Sheet for Quiz 13 2020

Stoichiometric Number	Name	$\Delta H^\circ_{f,298}$ (kJ/mol)	$\Delta G^\circ_{f,298}$ (kJ/mol)	Constants for C_P in J/mol-K a	b	c	d
-2	H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08
1	O2	0	0	28.11	-3.70E-06	1.75E-05	-1.07E-08
2	SO2	-296.8	-300.14	23.85	6.699E-02	-4.610E-05	1.328E-08
2	H2O	-242	-229	32.24	1.924E-03	1.055E-05	3.596E-09
0	I2 (g)	62.42	-15.27	37.79	2.214E-04	-9.126E-07	1.035E-09
0	HI	26.5	-34.9	29.05	4.690E-03	4.912E-06	-2.654E-09
0	H2	0	0	27.14	9.274E-03	-1.381E-05	7.645E-09

enter all species above line 14

Reaction T(K)	1103	P, bar
ΔH°_T (kJ/mol)	385.997	1
ΔG°_T (kJ/mol)	-156.990	
ln K_a	17.11831199	
K_a	27188699.6	

Intermediate Calculations, J and I defined in text

Δa	Δb	Δc	Δd
45.7116	-2.428E-01	2.426E-04	-6.463E-08

R (kJ/mol-K)	0.0083145
ΔH°_{298} (kJ/mol)	403.536
ΔG°_{298} (kJ/mol)	248.658
ln $K_{a,298}$	-100.30739
J (kJ/mol)	398.68458
I	-33.134308

Rxn 1	
Rxn Coord	Test
1.000033613	1137751.337

d) **0.209 bar**

Kcalc Sheet for Quiz 13 2020

Stoichiometric Number	Name	$\Delta H^\circ_{f,298}$ (kJ/mol)	$\Delta G^\circ_{f,298}$ (kJ/mol)	Constants for C_p in J/mol-K: a	b	c	d
-2	H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08
1	O2	0	0	28.11	-3.70E-06	1.75E-05	-1.07E-08
2	SO2	-296.8	-300.14	23.85	6.699E-02	-4.610E-05	1.328E-08
2	H2O	-242	-229	32.24	1.924E-03	1.055E-05	3.596E-09
0	I2 (g)	62.42	-15.27	37.79	2.214E-04	-9.126E-07	1.035E-09
0	HI	26.5	-34.9	29.05	4.690E-03	4.912E-06	-2.654E-09
0	H2	0	0	27.14	9.274E-03	-1.381E-05	7.645E-09

enter all species above line 14

Reaction T(K)	800	P, bar
ΔH°_T (kJ/mol)	392.335	0.209369295
ΔG°_T (kJ/mol)	-6.952	
ln K_a	1.045224105	
K_a	2.844035816	

Rxn 1	
Rxn Coord	Test
0.99	-0.000191809

Intermediate Calculations, J and I defined in text

Δa	Δb	Δc	Δd
45.7116	-2.428E-01	2.426E-04	-6.463E-08

R (kJ/mol-K)	0.0083145
ΔH°_{298} (kJ/mol)	403.536
ΔG°_{298} (kJ/mol)	248.658
ln $K_{a,298}$	-100.30739
J (kJ/mol)	398.68458
I	-33.134308

e) **0.909**

Kcalc Sheet for Quiz 13 2020

Stoichiometric Number	Name	$\Delta H^\circ_{f,298}$ (kJ/mol)	$\Delta G^\circ_{f,298}$ (kJ/mol)	Constants for C_P in J/mol-K a	b	c	d
-2	H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08
1	O2	0	0	28.11	-3.70E-06	1.75E-05	-1.07E-08
2	SO2	-296.8	-300.14	23.85	6.699E-02	-4.610E-05	1.328E-08
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0	I2 (g)	62.42	-15.27	37.79	2.214E-04	-9.126E-07	1.035E-09
0	HI	26.5	-34.9	29.05	4.690E-03	4.912E-06	-2.654E-09
0	H2	0	0	27.14	9.274E-03	-1.381E-05	7.645E-09

enter all species above line 14

			Intermediate Calculations, J and I defined in text Δa	Δb	Δc	Δd
Reaction T(K)	800	P, bar	45.7116	-2.428E-01	2.426E-04	-6.463E-08
ΔH°_T (kJ/mol)	392.335	1	R (kJ/mol-K)		0.0083145	
ΔG°_T (kJ/mol)	-6.952		ΔH°_{298} (kJ/mol)		403.536	
ln K_a	1.045224105		ΔG°_{298} (kJ/mol)		248.658	
K_a	2.844035816		ln $K_{a,298}$		-100.30739	
			J (kJ/mol)		398.68458	
			I		-33.134308	

Rxn 1	
Rxn Coord	Test
0.99	307.0168786

Part e) Reaction 1

	DG formation at 800K kJ/mole	n	y	nG/RT	nln(yP)
H2SO4	-537.03	0.181803549	0.0384583	-14.67915	-0.592349
O2	-8.803	0.909098225	0.1923083	-1.2032102	-1.4987895
SO2	-318.745	1.818196451	0.3846167	-87.133303	-1.7373013
H2O	-217.361	1.818196451	0.3846167	-59.418601	-1.7373013
		4.727294676	1	-162.43426	-5.5657412
	Rxn. Coord	4.727294676		G/RT	
	0.909098			-168.00001	