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:

$$2 \operatorname{H}_2 \operatorname{SO}_4(g) \Leftrightarrow \operatorname{O}_2(g) + 2 \operatorname{SO}_2(g) + 2 \operatorname{H}_2 \operatorname{O}(g) \qquad \qquad \text{Reaction (1)}$$

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 H₂SO₄. 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	Τ, Κ	P, bar
a)	0.99		1
b)	0.999		1
c)			1
d)	0.99		
e)		800	1

Your Name:_____

Answers

	Conversion of H2SO4	Т, К	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						
	ΔH ^o _{1,298}	ΔG ⁰ _{1,298}	Constants for Cp in J/mol-K				
Name	(kJ/mol)	(kJ/mol)	а	b	C	d	
H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08	
02	0	0	28.11	-3.70E-06	1.75E-05	-1.07E-08	
SO2	-296.8	-300.14	23.85	6.699E-02	-4.610E-05	1.328E-08	
H2O	-242	-229	32.24	1.924E-03	1.055E-05	3.596E-09	
l2 (g)	62.42	-15.27	37.79	2.214E-04	-9.126E-07	1.035E-09	
HI	26.5	-34.9	29.05	4.690E-03	4.912E-06	-2.654E-09	
H2	0	0	27.14	9.274E-03	-1.381E-05	7.645E-09	
above line 14			Intermediate Calculations, J and I defined in text			n text	
			Δa	ΔD	ΔC	Δd	
869.286735	P, bar		45.7116	-2.428E-01	2.426E-04	-6.463E-08	
390.569	1		R (kJ/mol-K)		0.0083145		
-41.459			ΔH ^o ₂₉₈ (kJ/mol)		403.536		
5.736123738			ΔG ^o 298 (kJ/mol)		248.658		
309.8609778			In K _{a,298}		-100.30739		
			J (kJ/mol)		398.68458		
			1		-33.134308		
Rxn 1							
Rxn Coord	Test						
0.00							
	Name H2SO4 O2 SO2 H2O I2 (g) HI H2 above line 14 869.286735 390.569 -41.459 5.736123738 309.8609778 Rxn 1 Rxn Coord	ΔH ⁰ (298) Name (kJ/mol) H2SO4 -740.568 O2 0 SO2 -296.8 H2O -242 I2 (g) 62.42 HI 26.5 H2 0 above line 14 26.5 Solution 1 390.569 1 -41.459 5.736123738 309.8609778 309.8609778 Rxn 1 Rxn Coord Rxn 1 2.00	Kcalc ΔH ^o t298 ΔG ^o t298 Name (kJ/mol) (kJ/mol) H2SO4 -740.568 -653.469 O2 0 0 SO2 -296.8 -300.14 H2O -242 -229 I2 (g) 62.42 -15.27 HI 26.5 -34.9 H2 0 0 above line 14	Kcalc Sheet for Quiz ΔH° _{1,298} ΔG° _{1,298} C Name (kJ/mol) (kJ/mol) a H2SO4 -740.568 -653.469 47.2892 O2 0 0 28.11 SO2 -296.8 -300.14 23.85 H2O -242 -229 32.24 I2 (g) 62.42 -15.27 37.79 HI 26.5 -34.9 29.05 H2 0 0 27.14 above line 14 Intermediate Ca ΔA 45.7116 390.569 1 R (kJ/mol-K) -41.459 ΔH° ₂₉₈ (kJ/mol) 5.736123738 ΔG° ₂₉₈ (kJ/mol) 309.8609778 In K _{a,298} J (kJ/mol) I Rxn 1 Es Rxn Coord Test	Kcalc Sheet for Quiz 13 2020 ΔH ⁰ ₁₂₉₈ ΔG ⁰ ₁₂₉₈ Constants for Quiz 13 2020 Name (kJ/mol) (kJ/mol) a b H2SO4 -740.568 -653.469 47.2892 1.903E-01 O2 0 0 28.11 -3.70E-06 SO2 -296.8 -300.14 23.85 6.699E-02 H2O -242 -229 32.24 1.924E-03 I2 (g) 62.42 -15.27 37.79 2.214E-04 HI 26.5 -34.9 29.05 4.690E-03 H2 0 0 27.14 9.274E-03 above line 14 Intermediate Calculations, J at Δa Δb above line 14 Intermediate Calculations, J at Δa Δb 390.569 1 R (kJ/mol/K) ΔG ⁰ ₂₈₆ (kJ/mol) 309.8609778 In K _{8,298} J (kJ/mol) I Rxn 1 Rxn 1 Rest Rest	Kcalc Sheet for Quiz 13 2020 ΔH ⁰ t298 ΔG ⁰ t298 Constants for C _P in J/mol-K Name (kJ/mol) (kJ/mol) a b c H2SO4 -740.568 -653.469 47.2892 1.903E-01 -1.481E-04 O2 0 0 28.11 -3.70E-06 1.75E-05 SO2 -296.8 -300.14 23.85 6.699E-02 -4.610E-05 H2O -242 -229 32.24 1.924E-03 1.055E-05 I2 (g) 62.42 -15.27 37.79 2.214E-04 -9.126E-07 H1 26.5 -34.9 29.05 4.690E-03 4.912E-06 H2 0 0 27.14 9.274E-03 -1.381E-05 above line 14 Intermediate Calculations, J and I defined i Δa Δb Δc above line 14 Intermediate Calculations, J and I defined i Δa Δb Δc above line 14 Intermediate Calculations, J and I defined i Δa Δb Δc Δc	

			Kcalo	Sheet for Quiz	13 2020		
Stoichiometric		ΔH ^o _{f,298}	ΔG° _{1,298}	C	onstants for (C _P in J/mol-K	
Number	Name	(kJ/mol)	(kJ/mol)	a	b	c	d
-4	2 H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08
1	02	0	0	28.11	-3.70E-06	1.75E-05	-1.07E-08
2	2 SO2	-296.8	-300.14	23.85	6.699E-02	-4.610E-05	1.328E-08
2	2 H2O	-242	-229	32.24	1.924E-03	1.055E-05	3.596E-09
() 12 (g)	62.42	-15.27	37.79	2.214E-04	-9.126E-07	1.035E-09
(HI	26.5	-34.9	29.05	4.690E-03	4.912E-06	-2.654E-09
	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			n text
				Δa	Δb	Δc	Δd
Reaction T(K)	951.0409964	P, bar		45.7116	-2.428E-01	2.426E-04	-6.463E-08
∆H° _T (kJ/mol)	388.687	1		R (kJ/mol-K)		0.0083145	
∆G° _T (kJ/mol)	-82.002			ΔH ^o ₂₉₈ (kJ/mol)		403.536	
n K _a	10.37028625			∆G° ₂₉₈ (kJ/mol)		248.658	
K _a	31897.60622			In K _{a,298}		-100.30739	
				J (kJ/mol)		398.68458	
				1		-33.134308	
	Rxn 1						
	Rxn Coord	Test					
	0 999	0.094875839					

c) 100% conversion

			Kcalo	Sheet for Quiz				
Stoichiometric		ΔH ^o _{1,298}	ΔG ⁰ 1,298	Constants for C _P in J/mol-K				
Number	Name	(kJ/mol)	(kJ/mol)	а	b	c	d	
-2	H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08	
1	02	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	l2 (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			n text	
				Δa	Δb	ΔC	Δd	
Reaction T(K)	1103	P, bar		45.7116	-2.428E-01	2.426E-04	-6.463E-08	
ΔH ^o T (kJ/mol)	385.997	1		R (kJ/mol-K)		0.0083145		
∆G ^o T (kJ/mol)	-156.990			ΔH ^o ₂₉₈ (kJ/mol)		403.536		
In K _a	17.11831199			ΔG ^o 298 (kJ/mol)		248.658		
Ka	27188699.6			In K _{a,298}		-100.30739		
				J (kJ/mol)		398.68458		
				1		-33.134308		
	Dvo 1							
	Ryn Coord	Toet						
	1.000033613	1137751,337						

d) **0.209 bar**

			Keale	Sheet for Quiz	13 2020		
			Real	, oneer for aquiz	10 2020		
Stoichiometric		ΔH ^o ₁₂₉₈	ΔG ⁰ 1298	Constants for C _P in J/mol-K			
Number	Name	(kJ/mol)	(kJ/mol)	а	b	c	d
-2	H2SO4	-740.568	-653.469	47.2892	1.903E-01	-1.481E-04	4.387E-08
1	02	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	l2 (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			n text
				Δa	Δb	Δc	Δd
Reaction T(K)	800	P, bar		45.7116	-2.428E-01	2.426E-04	-6.463E-08
ΔH ^o _T (kJ/mol)	392.335	0.209369295		R (kJ/mol-K)		0.0083145	
ΔG° _T (kJ/mol)	-6.952	I		ΔH ^o ₂₉₈ (kJ/mol)		403.536	
In Ka	1.045224105			∆G° ₂₉₈ (kJ/mol)		248.658	
Ka	2.844035816			In K _{a,298}		-100.30739	
				J (kJ/mol)		398.68458	
				1		-33.134308	
	Rxn 1						
	Rxn Coord	Test					
	0.99	-0.000191809					

e) **0.909**

			Kcalo	Sheet for Quiz	13 2020		
Stoichiometric		AH ⁰	AG ⁰	-	onetante for (C in I/mol-K	
Number	Nama	ΔΠ <u>(298</u>	//c //mell	0	b	op in J/mork	4
Number	Name H2SO4	740 568	(KJ/IIIOI)	47 2802	1 003E-01	1 4815-04	4 3875.08
	02	-740.508	-055.409	47.2032	-3 70E-06	1 75E-05	4.307E-08
2	802	206.8	-200.14	20.11	6.600E-00	4 610E-05	1.2285.08
2	302 H2O	-230.0	-300.14	23.00	1.039E-02	4.010E-05	2.5085.00
	12 (a)	-242	-223	32.24	2.214E-04	0.126E-07	1.035E-00
0	12 (g)	28.5	-13.27	20.05	4 800E-03	4.012E-06	2.654E-00
0		20.0	-34.9	23.00	4.030E-03	4.912E-00	7.845E-00
	112	0	0	27.14	9.274E-03	-1.301E-05	7.045E-09
enter all species	above line 14			Intermediate Ca	lculations, J a	nd I defined i	n text
				Δa	Δb	Δc	Δd
Reaction T(K)	800	P, bar		45.7116	-2.428E-01	2.426E-04	-6.463E-08
ΔH ^o T (kJ/mol)	392.335	1		R (kJ/mol-K)		0.0083145	
ΔG° _T (kJ/mol)	-6.952			ΔH° ₂₉₈ (kJ/mol)		403.536	
In K _a	1.045224105			∆G° ₂₉₈ (kJ/mol)		248.658	
Ka	2.844035816			In K _{a,298}		-100.30739	
				J (kJ/mol)		398.68458	
				1		-33.134308	
	Rxn 1						
	Rxn Coord	Test					
	0.99	307.0168786					
		Part e)	Reaction 1				
			DG form-				
			ation at	n	v	nG/RT	nin(vP)
			800K				
			kJ/mole				
		H2SO4	-537.03	0.181803549	0.0384583	-14.67915	-0.592349
		02	-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	
							T I