Homework #3A – MAE 640 **Rev 2023-01**

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Note: Also upload copies of any software used in these calculations that you have written.

Summary of Results

Result	SP03A_A	SP03A_B	Prob. 5.4	Prob. 5.11 Using CEQUEL	Comment on Reasons for Any Differences
T_c, [K]	5163	3500	3584.5	3627.95	5.4 was a lot of hand calculations which most likely introduced error
"x" for H_2O [-]	1	4.387	.64959	0.699738	Slight alterations in code convergence changed the final values
"x" for O_2 [-]	NA	2.54048	0.05078	0.035171	Slight alterations in code convergence changed the final values
"x" for H_2 [mole]	NA	1.27	0.16736	0.117764	Slight alterations in code convergence changed the final values
"x" for OH [-]	NA	NA	0.13204	0.097702	Slight alterations in code convergence changed the final values
"x" for Other	NA	NA	NA		
"x" for Other	NA	NA	NA		
γ	1.194	1.21	1.06195	1.125887	5.4 was a lot of hand calculations which most likely introduced error
$\boldsymbol{M}$ ($kg/kgmole$)	18	15.36	15.8977	15.69372	
c^* (m/s)	2381	2116.8	1328.6	2187	5.4 was a lot of hand calculations which most likely introduced error
Other	NA	NA	NA	NA	
Isp, vac for area ration of 10					

- ***Note the products are expressed in mole fraction and not moles in this***

Final Chemical Equation for SP03A_A

$$2H_2 + O_2 \rightarrow 2H_2O$$

Final Chemical Equation for SP03A_B

$$2H_2 + O_2 \rightarrow 1.266H_2O + 0.367O_2 + 0.734H_2$$

Final Chemical Equation for Prob. 5.4

$$2H_2 + O_2 \rightarrow 1.471H_2O + 0.115O_2 + 0.379H_2 + 0.299OH$$

Final Chemical Equation for Prob. 5.11

$$2H_2 + O_2 \rightarrow 1.854H_2O + 0.0932O_2 + 0.31209H_2 + 0.2589OH$$

Note any of the previous homework problems that you would like to have additional discussion on in lecture or helps sessions.

Special Problem *SP-03B-C*

Review your work on all the previous homework assignments compared with the solutions provided online. Complete the assessment below. First, do your own assessment of how well you currently understand the problem. Then compare your solutions with the instructor-provided solutions. If there are specific questions that remain, the type them in the space provided AND in the CANVAS Discussion Board.

	Self-Assessment of Submission			**Self-Assessment after Reviewing Solution**			
HW Problem	Good	Ave	Poor	Good	Ave	Poor	Specific Questions That you would like answered about problems. Also Put these questions in the CANVAS Test 01 Homework Review Discussion Board with Homework Submission
2.6	X			X			
3.8	X			X			
4.24	X			X			
4.30	X			X			
01SP_A	X						
01SP_B			X		X		
01SP_C		X			X		
11.3	X			X			
11.17	X			X			
02-A_SPA	X			X			
02-A_SPB	X			X			
11.4	X			X			
SP02-B_A	X			X			
SP03A_A		X			X		
SP03A_B		X			X		

Other							

General Instructions

- Uploading Assignment: The entire homework assignment must be uploaded in the CANVAS drop box in one file. Use the filename *xxHW_Lastname_revxx.doc* when uploading to CANVAS. Your homework must be written neatly or typed. If you want to write it out, you can scan it or take pictures of it with your phone (tinyscan for phones works). I must be able to read the uploaded file. Submitting all solutions in one file is required.
- Uploading spreadsheets or other programs: If you use spreadsheets or other programs, put in screenshots of your graphs or pertinent tables into your homework file submission. You do not have to upload your spreadsheets, videos, or programs unless specifically requested in the assignment sheet. When using computer programs, be sure to document in your homework submission the basic equations and example calculations with units showing how the program works.
- Re-submitting homework: If you submit your package and then resubmit an update before the deadline, the newest submission will be graded.
- Grading Rubric**:** The homework grading rubric is shown on CANVAS. The completeness of the entire homework package is also a component of the homework grade.

Assigned Problems:

- Textbook Problems

Required Homework Format (See Example at end of this Syllabus)

In the solution of problems, you are required to:

1. **Name:** Provide name of the student.
2. **Given**: State briefly and concisely (in your own words) the information provided.
3. **Find:** State the information that you have to find.
4. **Schematic**: Draw a schematic representation of the system and control volume if applicable.
5. **Assumptions:** List the simplifying assumptions that are appropriate to the problem and implied by the equations used.
6. **Basic Equations**: Outline the basic equations needed to do the analysis. Use the proper symbol from the book where applicable.
7. **Analysis:** Manipulate the basic equations to the point where it is appropriate to substitute numerical values. Substitute numerical values (using a consistent set of units) to obtain a numerical answer. Include appropriate units in calculations. If multiple repetitive calculations are done on a spreadsheet for example, show at least one example calculation in detail, including all units. The significant figures in the answer should be consistent with the given data. Check the answer and the assumptions made in effecting the solution to make sure they are reasonable.
8. **Answer**. Label the answer(s) with a box and an arrow from the right-hand margin.
9. **Comment**: Write a comment at the end of the homework that reflects on the limitations of the solution, the reasonableness of the solution, or something that you learned by doing the problem.

All nine formatting elements must be specifically shown in Each HW to receive full credit unless otherwise specified.

Name:

Veronica Loomis

Problem 5.4

Given: $2H_2 + O_2 \rightarrow aH_2O + bO_2 + cH_2 + dOH$

And dissociation reactions

$H_2 + \frac{1}{2}O_2 \leftrightharpoons H_2O$ and $\frac{1}{2}O_2 + \frac{1}{2}H_2 \leftrightharpoons OH$

Find: Balanced chemical equation, molecular weight, characteristic velocity, and specific heat ratio, and adiabatic flame temp

Assumptions: Reactants are at 298K & P = 50 atm

Include temp dependent C_p data from T5.3

Using Purdue's K_p table

Basic Equations:

$$H = h^\circ + \int C_p \, dT$$

$$\gamma = \frac{C_p}{C_p - R_u}$$

$$c^* = \sqrt{\frac{R_u T_c}{\gamma M}}$$

Analysis:

$$2H_2 + O_2 \rightarrow aH_2O + bO_2 + cH_2 + dOH$$

H: $4 = 2a + 2c + d$

O: $2 = a + 2b + d$

$d = 2 - a - 2b$

Sub into H's

$4 = 2a + 2c + 2 - a - 2b$

$2c = 2 - a + 2b$

$c = 1 - \frac{1}{2}a + b$

Rewrite chemical eq

$$2H_2 + O_2 \rightarrow aH_2O + bO_2 + (1 - \tfrac{1}{2}a + b)H_2 + (2 - a - 2b)OH$$

So, the total number of moles is

$n = a + b + 1 - \frac{1}{2}a + b + 2 - a - 2b$

$n = -\frac{1}{2}a + 3$

We also have

$$K_{p,3} = \frac{\chi_{OH}}{\sqrt{\chi_{O_2}}\,\chi_{H_2}} P^{(1 - 1/2 - 1/2)}$$

$$K_{p,4} = \frac{\chi_{H_2O}}{\chi_{H_2}\sqrt{\chi_{O_2}}} P^{(1 - 1 - 1/2)}$$

$$\chi_{H_2O} = \frac{a}{-\frac{1}{2}a + 3}, \quad \chi_{H_2} = \frac{1 - \frac{1}{2}a + b}{-\frac{1}{2}a + 3}, \quad \chi_{O_2} = \frac{b}{-\frac{1}{2}a + 3}, \quad \chi_{OH} = \frac{2 - a - 2b}{-\frac{1}{2}a + 3}$$

$$K_{p3} = \frac{\frac{2 - a - 2b}{-\frac{1}{2}a + 3}}{\left(\frac{b}{-\frac{1}{2}a + 3}\right)^{1/2}\left(\frac{1 - \frac{1}{2}a + b}{-\frac{1}{2}a + 3}\right)^{1/2}} = \frac{2 - a - 2b}{(b + b^2 - \frac{1}{2}ab)^{1/2}}$$

$$K_{p4} = \frac{\frac{a}{-\frac{1}{2}a + 3}}{\left(\frac{1 - \frac{1}{2}a + b}{-\frac{1}{2}a + 3}\right)\left(\frac{b}{-\frac{1}{2}a + 3}\right)^{1/2}} P^{-1/2} = \frac{a(-\frac{1}{2}a + 3)^{1/2}}{b^{1/2}(1 - \frac{1}{2}a + b)} P^{-1/2}$$

Reactants = 0 since $h^\circ = 0$ for both H_2 & O_2 and they are injected at 298K

Products:

$$0 = a\left[-57800 \frac{cal}{mol}(4.184)\frac{J}{cal} + \int_{298}^{T_c} C_p\,dT\right]_{H_2O} + b\left[\int_{298}^{T_c} C_p\,dT\right]_{O_2}$$

$$+ (1 - \tfrac{1}{2}a + b)\left[\int_{298}^{T_c} C_p\,dT\right]_{H_2} + (2 - a - 2b)\left[10060 \frac{cal}{mol}(4.184)\frac{J}{cal} + \int_{298}^{T_c} C_p\,dT\right]_{OH}$$

$$Cp_{H_2O} = 29.182 + 14.503\,(T/1000) - 2.0235\,(T/1000)^2$$

$$Cp_{O_2} = 28.186 + 6.3011\,(T/1000) - 0.74436\,(T/1000)^2$$

$$Cp_{H_2} = 26.896 + 4.3501\,(T/1000) - 0.32674\,(T/1000)^2$$

$$Cp_{OH} = 81.55 - 15\,(T)^{1/4} + 0.313\,(T)^{3/4} - 0.02\,(T)$$

$\frac{J}{gmol\,K}$

Plug these in to enthalpy balance, guess Tc, check Kp, get a & b, determine $H_1 = H_2$. Iterate & repeat

For P = 50 atm,

$T_c = 3584.517\,K$

$a = 1.471,\ b = 0.115,\ c = 0.379,\ d = 0.299$

$$2H_2 + O_2 \rightarrow 1.471\,H_2O + 0.115\,O_2 + 0.379\,H_2 + 0.299\,OH$$

$$M = \frac{1.471}{-\frac{1}{2}(1.471)+3}(18) + \frac{0.115}{-\frac{1}{2}(1.471)+3}(32) + \frac{0.379}{\frac{1}{2}(1.471)+3}(2) + \frac{0.299}{\frac{1}{2}(1.471)+3}(17)$$

$M = 15.898\ g/gmol$

Specific heat ratio

$$\gamma = \frac{Cp}{Cp - R_u}$$

Cp total (excel) = 142.517 J/gmolK

$$\gamma = \frac{142.5}{142.5 - 8.317}$$

$\gamma = 1.06195$

Char vel

$$C^* = \sqrt{\frac{R_u T_c}{\gamma M}} = \sqrt{\frac{8.314\ \frac{Nm}{gmol\,K} \times 3584.5K \times 1000\,g/kg}{1.06195 \times 15.898\ g/gmol}}$$

$C^* = 1328.6\ m/s$

Want:				Given	T0	298	K
a	1.471162787				P	50	atm
b	0.11491999						
c	0.379338596						
d	0.298997234						
		(T/1000)	(T/1000)^2				
CpH2O	29.182	14.503	-2.0235				
CpO2	28.186	6.3011	-0.74986				
CpH2	26.896	4.3501	-0.32674				
		T^(-0.25)	T^(-0.75)	T			
CpOH	81.55	-15.01	0.313	-0.02			

to get a and b

a	b	kp3	kp4	constraint
1.471162787	0.11491999	1.432042359	3.663596	0.043594

Tc	Kp3	Kp4	a	b	enthH2O	enthO2	enthH2	enthOH	enth_sum
3584.516761	1.432042359	3.663596384	1.471163	0.11492	-79461	15918.64	48882.09	14660.3	9.31512E-07

n	2.264418607		
0.649614871	0.050785663	0.16737188	0.132043
molecular weight	15.89767894		

all Cp	
h20	55.1687799
o2	41.13762708
h20	38.29080239
oh	7.920468592
cp_total	142.517678
gamma	1.061950612

c*	1328.605425

	O2(G) H2(G)	
OF=	7.936508	7.936508
Pc (bar)	50.6625	50.6625
Area Ratio	0	1

		CEQUEL calculations		Pasted Values	
OF	DIMENSIONLESS	#NAME?	#NAME?	7.936508	7.936508
FPCT	DIMENSIONLESS	#NAME?	#NAME?	11.19005	11.19005
ERATIO	DIMENSIONLESS	#NAME?	#NAME?	1.000022	1.000022
Phi	DIMENSIONLESS	#NAME?	#NAME?	1.000022	1.000022
AR	DIMENSIONLESS	#NAME?	#NAME?	0	1
P	BAR	#NAME?	#NAME?	50.6625	29.35265
T	DEG K	#NAME?	#NAME?	3627.95	3458.989
RHO	KG/M^3	#NAME?	#NAME?	2.635812	1.624421
H	KJ/KG	#NAME?	#NAME?	0.00025	-1017.21
U	KJ/KG	#NAME?	#NAME?	-1922.08	-2824.17
GFE	KJ/KG	#NAME?	#NAME?	-58426.8	-56723
S	KJ/(KG K)	#NAME?	#NAME?	16.10464	16.10464
Z	DIMENSIONLESS	#NAME?	#NAME?	1	1
MW	MOL WT	#NAME?	#NAME?	15.69372	15.91612
CP	KJ/(KG K)	#NAME?	#NAME?	11.25069	11.07433
CPG	KJ/(KG K)	#NAME?	#NAME?	3.247882	3.225807
GammaG	DIMENSIONLESS	#NAME?	#NAME?	1.194916	1.193236
Gamma	DIMENSIONLESS	#NAME?	#NAME?	1.129392	1.125887
C	M/S	#NAME?	#NAME?	1473.359	1426.335
MW_MIX	MOL WT	#NAME?	#NAME?	15.69372	15.91612
Viscosity	milliPOISE	#NAME?	#NAME?	1.129003	1.089942
Specific_Heat_Eq	KJ/(KG K)	#NAME?	#NAME?	11.2511	11.07453
Conductivity_Eq	milliW/(CM K)	#NAME?	#NAME?	24.71064	23.44813
Prandtl_Eq	DIMENSIONLESS	#NAME?	#NAME?	0.514051	0.514779
Specific_Heat_Fr	KJ/(KG K)	#NAME?	#NAME?	3.247949	3.22585
Conductivity_Fr	milliWATTS/(CM K)	#NAME?	#NAME?	5.065193	4.812006
Prandtl_FR	DIMENSIONLESS	#NAME?	#NAME?	0.72395	0.73067
PINJ_P	N/A	#NAME?	#NAME?	-999.999	-999.999
PC_P	DIMENSIONLESS	#NAME?	#NAME?	1	1.725994
MACH	DIMENSIONLESS	#NAME?	#NAME?	0	0.999997
AR	DIMENSIONLESS	#NAME?	#NAME?	0	1
CSTAR	M/S	#NAME?	#NAME?	0	2187
CF	DIMENSIONLESS	#NAME?	#NAME?		0.652309
ISPV	M/S	#NAME?	#NAME?		2693.19
ISP	M/S	#NAME?	#NAME?		1426.332
ISPVRHO	KG/(M^2 S)	#NAME?	#NAME?		0
H2	MOLE	#NAME?	#NAME?	0.12661	0.117764
H2O	MOLE	#NAME?	#NAME?	0.670352	0.699738
O2	MOLE	#NAME?	#NAME?	0.036608	0.035171
OH	MOLE	#NAME?	#NAME?	0.108989	0.097702