

**This Homework Must Be Uploaded onto CANVAS to Receive Credit.
Deadline: Shown in Syllabus**

Name: _____

General Instructions

- **Uploading Assignment:** The entire homework assignment must be uploaded in the CANVAS dropbox 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. 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.

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

In the solution of problems, you are required to:

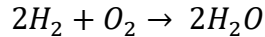
1. **Name:** Provide name of the student.
2. **Given:** State briefly and concisely (in your own words) the information provided.
3. **Find:** State the information that you have to find.
4. **Schematic:** Draw a schematic representation of the system and control volume if applicable.
5. **Assumptions:** 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.

Special Problem SP-03A-A

1. **Name:** Robert Frederick

2. **Given:** Example problem in textbook section 5.4.1:

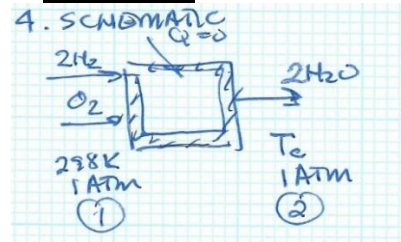


Adiabatic, no dissociation, $P = 1 \text{ atm}$

3. **Find:**

- Adiabatic flame temperature $T_{adiabatic}$
- Coefficient of the products, a
- Molecular weight of the products, $M_{product}$
- Specific heat ratio of the products, $\gamma_{product}$
- Characteristic velocity of the products, $c^*_{products}$
- Plot of specific heat of water as a function of temperature
- Plot of total enthalpy as a function of temperature (+5 Points Bonus)

4. **Schematic:**



5. **Assume:**

- Adiabatic combustion
- No dissociation
- Heats of Formation from Table 5.1
- Specific heat fits from Table 5.3
- Constant pressure, 1 atm
- Reactant temperature = 298 K
- Steady state, No work, No ΔKE , No ΔPE

6. **Basic Equations:**

$$\Delta H = 0 = \sum_{i=1}^n b_i \left(\int_{T^0}^T C_{p_{B,i}} dT + h_{B,i}^0 \right) - \sum_{j=1}^n a_j \left(\int_{T^0}^T C_{p_{A,j}} dT + h_{A,j}^0 \right) \quad (5.31)$$



$$\bar{c}_p = a + b(T/1000) + c(T/1000)^2 + d(T/1000)^3 \quad J/mol \cdot K$$

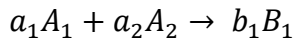
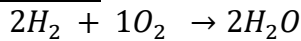
$$H_2O \rightarrow a = 29.182, b = 14.503, c = -2.0235, d = 0 \quad [\text{Range} = 273-3770K]$$

$$\Delta \bar{h}_{f,H_2}^0 = 0 \quad \Delta \bar{h}_{f,O_2}^0 = 0 \quad \Delta \bar{h}_{f,H_2O(g)}^0 = -57.7979 \text{ kcal/mol}$$

$$\Delta \bar{h}_{f,H_2O(v)}^0 = -57.7979 \frac{\text{kcal}}{\text{mole}} \left(\frac{1000 \text{ cal}}{\text{kcal}} \right) \left(\frac{4.184}{\text{cal}} \right) = -241,826.41 \text{ J/mol}$$

$$\gamma = \frac{\bar{c}_p}{\bar{c}_p - R_u} \quad c^* = \frac{P_c A_t}{\dot{m}} = \sqrt{\frac{R_u T_c}{\gamma M_{mix}}} \left(\frac{2}{\gamma+1} \right)^{\frac{-(\gamma+1)}{2(\gamma-1)}} \quad (4-29)$$

7. Analysis:



$$a_1 = 2 \text{ moles}, A_1 = H_2$$

$$a_2 = 1 \text{ moles}, A_2 = O_2$$

$$b_1 = 2 \text{ moles}, B_1 = H_2O$$

$$\Delta H = H_2 - H_1 = 0$$

$$0 = b_1 \left(\int_{T^0}^{T_2} C_{p_{B1}} dT + h_{B1}^o \right) - a_1 \left(\int_{T^0}^{T_1} C_{p_{A1}} dT + h_{A1}^o \right) - a_2 \left(\int_{T^0}^{T_1} C_{p_{A2}} dT + h_{A2}^o \right)$$

$$h_{H_2O(v)}^o = -57.7979 \frac{\text{kcal}}{\text{mole}} \left(\frac{1000 \text{ cal}}{\text{kcal}} \right) \left(\frac{4.184 \text{ J}}{\text{cal}} \right) = -241,826.41 \text{ J/mol}$$

$$h_{H_2(g)}^o = 0$$

$$h_{O_2(g)}^o = 0$$

$$\text{Since } T_1 = T_0, \int_{T^0}^{T_1} C_{p_{A1}} dT = \int_{T^0}^{T_1} C_{p_{A2}} dT = 0 \text{ for the reactants}$$

$$C_{p,H_2O} = a + b(T/1000) + c(T/1000)^2 + d(T/1000)^3$$

$$\text{From Table 5.3 for } H_2O(\text{gas}), a = 29.182, b = 14.503, c = -2.0235, d = 0$$

So integrating first,

$$b_1 \left\{ \int_{T^0}^{T_2} [a + b(T/1000) + c(T/1000)^2] dT + h_{f,H_2O}^o \right\} = 0$$

$$b_1 \left\{ aT + \frac{bT}{2} \left(\frac{T}{1000} \right) + \frac{cT}{3} \left(\frac{T}{1000} \right)^2 \right|_{T^0}^{T_2} + h_{f,H_2O}^o \right\} = 0$$

$$b_1 \left\{ \left[aT_2 + \frac{bT_2}{2} \left(\frac{T_2}{1000} \right) + \frac{cT_2}{3} \left(\frac{T_2}{1000} \right)^2 \right] - \left[aT^0 + \frac{bT^0}{2} \left(\frac{T^0}{1000} \right) + \frac{cT^0}{3} \left(\frac{T^0}{1000} \right)^2 \right] + h_{f,H_2O}^o \right\} =$$

$$H_2 - H_1 = 0$$

Sample Calculation

1. Put in coefficients
2. Guess T_2
3. Calculate $H_2 - H_1$
4. Iterate on temperature until $H_2 - H_1 = 0$

Example Guessing $T_2 = 3000\text{K}$

$$\begin{aligned} & 2 \text{ moles} \left[29.182(3000) + \frac{14.503(3000)}{2} \left(\frac{3000}{1000} \right) + \frac{-2.0235(3000)}{3} \left(\frac{3000}{1000} \right)^2 \right] \text{ J/mole} \\ & - 2 \text{ moles} \left[29.182(298) + \frac{14.503(298)}{2} \left(\frac{298}{1000} \right) + \frac{-2.0235(298)}{3} \left(\frac{298}{1000} \right)^2 \right] \text{ J/mole} \end{aligned}$$

$$\begin{aligned}
 &+ 2\text{moles} \left[-241864 \frac{\text{J}}{\text{mol}} \right] = H_2 - H_1 \\
 \Rightarrow & 2\text{moles}[87546 + 65263.5 - 18211.5] \text{ J/mole} \\
 &- 2\text{moles}[8696.236 + 643.962 - 17.85] \text{ J/mole} \\
 &+ 2\text{moles} \left[-241826.41 \frac{\text{J}}{\text{mol}} \right] = H_2 - H_1 \\
 \Rightarrow & H_2 - H_1 = 269,196 \text{ J} - 18,644.7 \text{ J} - 483,652.8 \text{ J} = -233,101.5 \text{ J}
 \end{aligned}$$

Comment: At the assumed product temperature of 3,000K, the change in enthalpy inside of the box assuming that H₂O is the only product is -233,202 J. This means that for the assumed product, we would have to take out 233kJ of heat from the control volume to get the gases to 3000K. The adiabatic temperature, Q = 0, is therefore much higher than 3000K.

Part a)

Iterating with spreadsheet, $T_{AF} = T_2 = 5163.24\text{K}$



Part b)

$$b_1 = 2 \text{ moles}$$



Part c)

$$M_{H_2O} = 16 \frac{\text{kg}}{\text{mol}} + 2 \frac{\text{kg}}{\text{mol}} = 18 \frac{\text{kg}}{\text{mol}}$$

$$\Rightarrow M_{H_2O} = 18 \frac{\text{kg}}{\text{kmol}}$$



Part d)

$$\gamma_{mix} = \frac{\bar{c}_{p,mix}}{\bar{c}_{p,mix} - R_u}$$

$$\bar{c}_{p,mix} = \bar{c}_p(5163.24\text{K}) = 29.182 + 14.503 \left(\frac{5163.24}{1000} \right) - 2.0235 \left(\frac{5163.24}{1000} \right)^2 = 50.12 \frac{\text{J}}{\text{mol-K}}$$

$$R_u = 8317 \frac{\text{J}}{\text{kmol-K}} \frac{\text{kmole}}{1000\text{mole-K}} = 8.317 \frac{\text{J}}{\text{mol-K}}$$

(Note the books value for R_u is incorrect. It should be $8,314.4598 \frac{\text{J}}{\text{kmol-K}}$)

$$\gamma_{mix} = \frac{50.12 \frac{\text{J}}{\text{mol-K}}}{50.12 \frac{\text{J}}{\text{mol-K}} - 8.317 \frac{\text{J}}{\text{mol-K}}} = 1.199 = 1.2$$

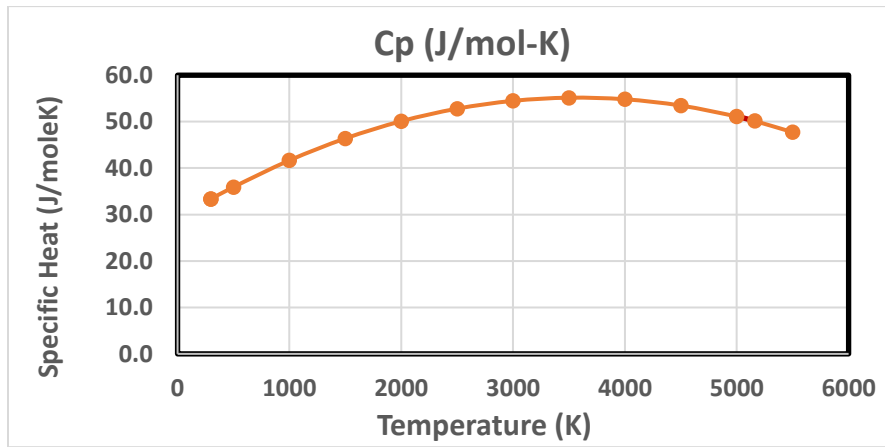


Part e)

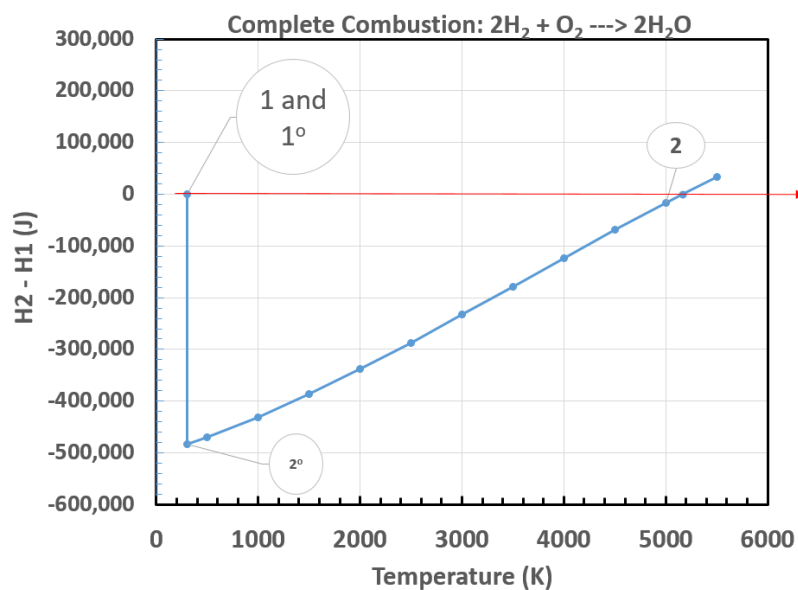
$$c^* = \sqrt{\frac{8.317 \frac{\text{J}}{\text{mol-K}} \frac{1000\text{mole}}{\text{kmole}} (5163.24\text{K}) \left(\frac{\text{Nm}}{\text{J}} \right) \left(\frac{\text{kg-m}}{\text{N-s}^2} \right)}{1.199 \times 18 \frac{\text{kg}}{\text{kmol}}} \left(\frac{2}{1.199+1} \right)^{\frac{-(1.199+1)}{2(1.199-1)}}$$

$$c^* = 2381 \text{ m/s}$$

Part f)



Part g)



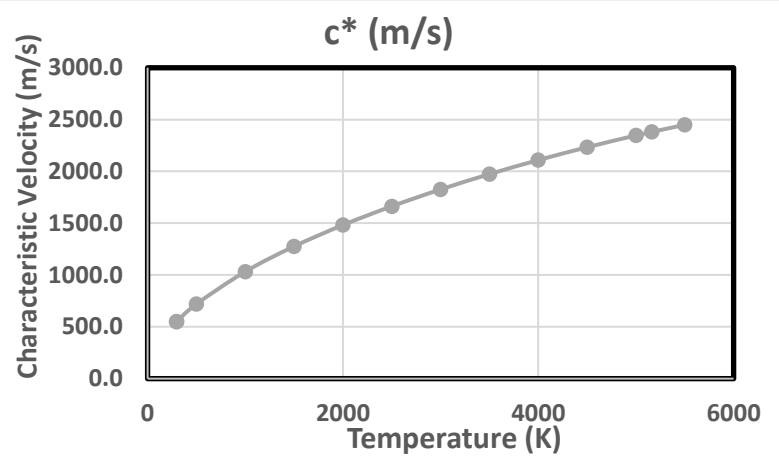
8. Answers:

- (a) $T_{AF} = 5163.24 \text{ K}$
- (b) $b_1 = 2 \text{ moles}$
- (c) $M_{H_2O} = 18 \frac{\text{kg}}{\text{kmol}}$
- (d) $\gamma_{mix} = 1.2$
- (e) $c^* = 2381 \text{ m/s}$

9. Comments:

Complete combustion greatly over-predicts the adiabatic flame temperature by not accounting for dissociation of the H_2O in the products.

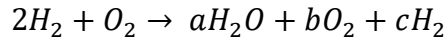
					H ₂ O(VAP)
M=	18.015	kg/kmole		a	29.182
b ₁ =	2	moles		b	14.503
h _{fg}	(241,826.41)	J/(mole*K)		c	-2.0235
H ₂₉₈	18,644.70	J/(mole*K)	CSD6:	d	0
Ru	8317	J/(kmoleK)			
T (K)	H ₂ - H ₁ (J)	C _p (J/moleK)	γ	c* (m/s)	
298.00	0.00	33.324	1.333	551.07	
298.00	-483,652.83	33.324	1.333	551.07	
500.00	-469,658.40	35.928	1.301	719.80	
1000.00	-430,779.52	41.662	1.249	1032.69	
1500.00	-386,672.65	46.384	1.218	1276.15	
2000.00	-338,349.52	50.094	1.199	1482.07	
2500.00	-286,821.90	52.793	1.187	1663.06	
3000.00	-233,101.52	54.480	1.180	1825.58	
3500.00	-178,200.15	55.155	1.178	1973.42	
4000.00	-123,129.52	54.818	1.179	2108.85	
4500.00	-68,901.40	53.470	1.184	2233.13	
5000.00	-16,527.52	51.110	1.194	2346.69	
5163.24	0.00	50.120	1.199	2381.40	
5500.00	32,980.35	47.738	1.211	2449.05	



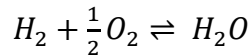
Special Problem SP-03A-B

1. **Name:** Robert Frederick

2. **Given:** Gaseous hydrogen and oxygen at 1 atm and $T = 298K$ with following reaction:



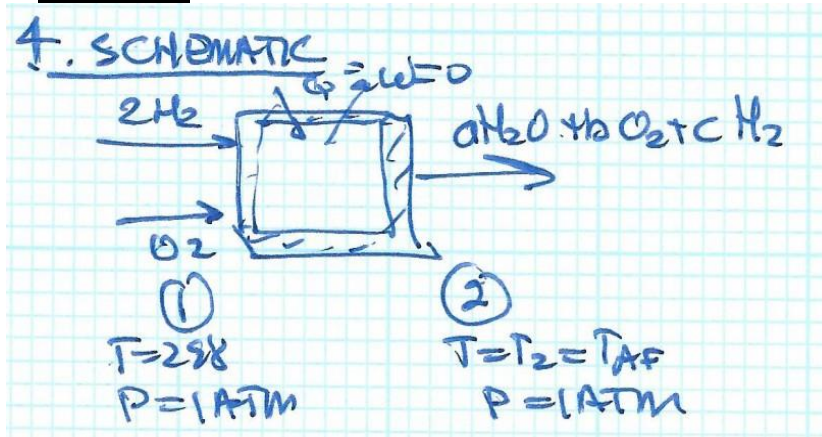
With the presumed products shown, considering the dissociation reaction:



3. **Find:**

- Adiabatic flame temperature $T_{adiabatic}$
- Coefficient of the products, a
- Molecular weight of the products, $M_{product}$
- Specific heat ratio of the products, $\gamma_{product}$
- Characteristic velocity of the products, $c^*_{products}$
- Plot of specific heat of H_2O , O_2 and H_2 as a function of temperature
- Plot of total enthalpy as a function of temperature (Bonus +5 Points)

4. **Schematic:**



5. **Assume:**

- Adiabatic combustion
- Limited dissociation
- Heats of Formation from Table 5.1
- Specific heat fits from Table 5.3
- Constant pressure
- Complete combustion
- Steady state

6. **Basic Equations:**

$$a_1A_1 + a_2A_2 \rightarrow b_1B_1 + b_2B_2 + b_3B_3 \quad (5.28)$$

$$H_2 - H_1 = 0 = \sum_{i=1}^n b_i \left(\int_{T^0}^T C_{p_{B,i}} dT + h_{B,i}^o \right) - \sum_{j=1}^n a_j \left(\int_{T^0}^T C_{p_{A,i}} dT + h_{A,i}^o \right) \quad (5.31)$$

$$K_p = \frac{X_{H_2O}}{X_{H_2} X_{O_2}^{1/2}} p^{1-1-\frac{1}{2}} \quad X_i = \frac{n_i}{\sum n_i} \quad (5.48)$$

$$M_{mix} = \sum X_i M_i \quad (5.15)$$

$$\gamma_{mix} = \frac{\bar{c}_{p_{mix}}}{\bar{c}_{p_{mix}} - R_u} \quad (5.7)$$

$$\bar{c}_{p_{mix}} = \sum X_i \bar{c}_{p_i} \quad (5.16)$$

$$c^* = \frac{P_c A_t}{\dot{m}} = \sqrt{\frac{R_u T_c}{\gamma M_{mix}}} \left(\frac{2}{\gamma+1} \right)^{\frac{-(\gamma+1)}{2(\gamma-1)}} \quad (4.29)$$

7. Analysis:

Setup

Atom Balance: $2H_2 + O_2 \rightarrow aH_2O + bO_2 + cH_2$

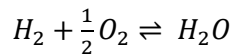
$$\text{H: } 2(2) = a(2) + b(2)$$

$$\text{O: } (2) = a + b(2)$$

$$2H_2 + O_2 \rightarrow aH_2O + \left(\frac{2-a}{2} \right) O_2 + (2-a)H_2$$

$$n = \sum n_i = a + \left(\frac{2-a}{2} \right) + (2-a) = \frac{6-a}{2}$$

Need additional equation from equilibrium constant,



$$K_p(T_2) = \frac{X_{H_2O}}{X_{H_2} X_{O_2}^{1/2}} p^{-1/2} \quad (\text{Note Pressure is in Atmospheres})$$

$$X_{H_2O} = \frac{2a}{6-a}$$

$$X_{H_2} = \frac{2-a}{6-a} * 2$$

$$X_{O_2}^{1/2} = \frac{2a}{2} * \frac{2}{6-a} = \frac{2-a}{6-a}$$

$$p^{-1/2} = \left(\frac{1 \text{ ATM}}{1 \text{ ATM}} \right)^{-1/2} = 1$$

$$\Rightarrow K_p(T_2) = \frac{\frac{2a}{6-a}}{\frac{2-a}{6-a} * 2 * \left(\frac{2-a}{6-a} \right)^{1/2}} = \frac{a(6-a)^{1/2}}{(2-a)^{3/2}}$$

Lookup $K_p(T_2)$ in Table 5.2 [Column $K_{p,4}$ noting that $K_{p,4}$ at 4000K is incorrect in the table (should be 1.6623)]

So, $\boxed{K_p(T_2) = \frac{a(6-a)^{1/2}}{(2-a)^{3/2}}}$ with the unknowns T_2, a

Energy equation now becomes,

Note the stoichiometric “a” and the curve fit “a” are different numbers

$$\begin{aligned}
 H_2 - H_1 &= a \left[\int_{298K}^{T_2} C_p dT + h_f^o \right]_{H_2O} + (2 - a) \left[\int_{298K}^{T_2} C_p dT + h_f^o \right]_{H_2} \\
 &\quad + \left(\frac{2-a}{2} \right) \left[\int_{298K}^{T_2} C_p dT + h_f^o \right]_{O_2} - 2 \left[\int_{298K}^{298K} C_p dT + h_f^o \right]_{H_2} - 1 \left[\int_{298K}^{298K} C_p dT + h_f^o \right]_{H_2} \\
 \Rightarrow H_2 &= a \left[a \left(\frac{T}{1000} \right) + \frac{bT}{2} \left(\frac{T}{1000} \right)^2 + \frac{cT}{3} \left(\frac{T}{1000} \right)^3 + \frac{dT}{4} \left(\frac{T}{1000} \right)^4 \right]_{T^0}^{T_2} + a \Delta h_f^o|_{H_2O} \\
 &\quad + (2 - a) \left[a \left(\frac{T}{1000} \right) + \frac{bT}{2} \left(\frac{T}{1000} \right)^2 + \frac{cT}{3} \left(\frac{T}{1000} \right)^3 + \frac{dT}{4} \left(\frac{T}{1000} \right)^4 \right]_{T^0}^{T_2} \Big|_{O_2} \\
 &\quad + \left(\frac{2-a}{2} \right) \left[a \left(\frac{T}{1000} \right) + \frac{bT}{2} \left(\frac{T}{1000} \right)^2 + \frac{cT}{3} \left(\frac{T}{1000} \right)^3 + \frac{dT}{4} \left(\frac{T}{1000} \right)^4 \right]_{T^0}^{T_2} \Big|_{H_2}
 \end{aligned}$$

Solution Technique

1. Guess T_2
2. Find K_p
3. Solve for a (*Stoichiometric coefficient*)
4. Put a in the energy equation
5. Solve for H_2
6. Check if $H_2 \approx 0$
7. Iterate on T_2 and repeat until the condition $H_2 \approx 0$ is true

Calculate,

$$M_{mix} = X_{H_2O} M_{H_2O} + X_{H_2} M_{H_2} + X_{O_2} M_{O_2}$$

$$\bar{C}_{p_{mix}} = X_{H_2O} \bar{C}_{H_2O} + X_{H_2} \bar{C}_{H_2} + X_{O_2} \bar{C}_{O_2}$$

$$\gamma = \frac{\bar{C}_{p_{mix}}}{\bar{C}_{p_{mix}} - R_u}$$

$$c^* = \sqrt{\frac{R_u T_c}{\gamma M_{mix}}} \left(\frac{2}{\gamma+1} \right)^{\frac{-(\gamma+1)}{2(\gamma-1)}}$$

$$\text{Input } \Delta h_f^o|_{H_2O} = -57.7879 \left(\frac{\text{kcal}}{\text{mol-K}} \right) \left(\frac{1000 \text{cal}}{\text{kcal}} \right) \left(4.184 \frac{\text{J}}{\text{cal}} \right) = 241.785 \frac{\text{J}}{\text{mol-K}}$$

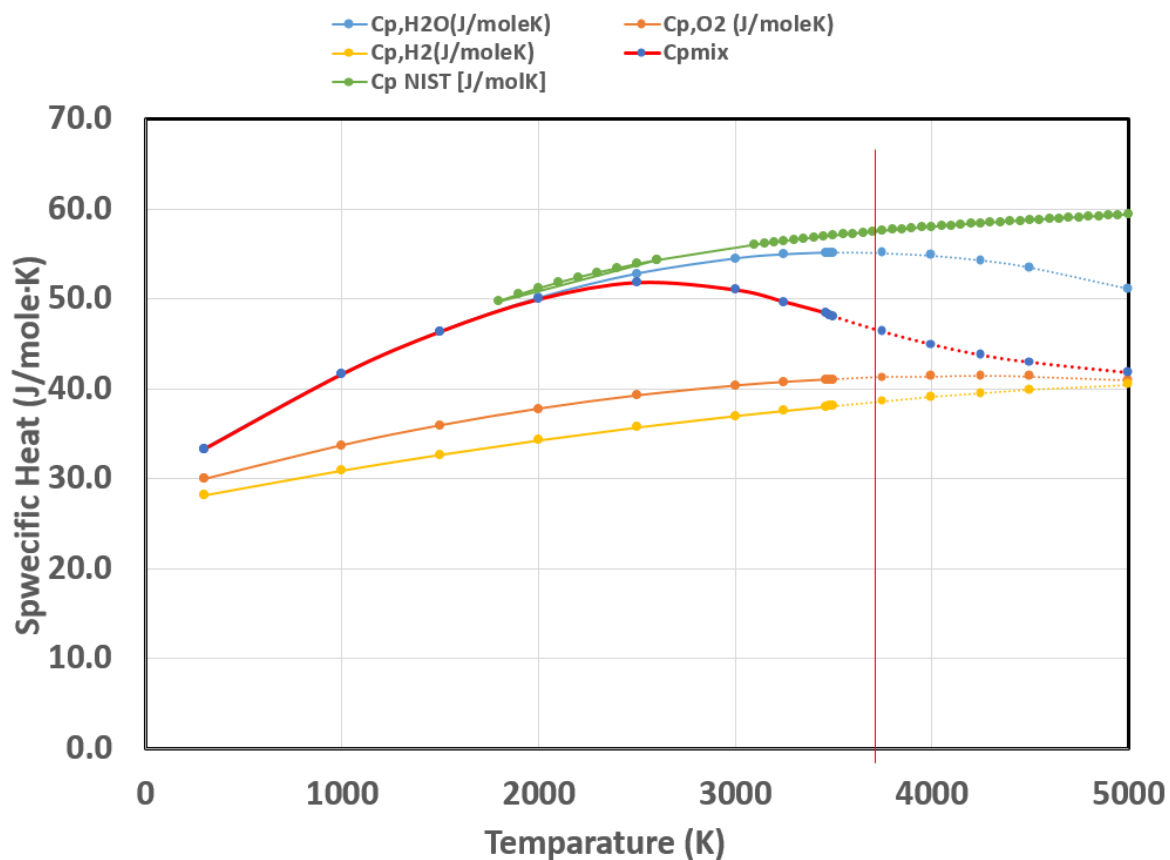
Assumed Specific Heat Curve Fit Coefficients (From Book)

	a	b	c	d
H_2O	29.182	14.503	-2.0235	0
H_2	26.896	4.3501	-0.32674	0
O_2	28.186	6.3011	-0.74986	0

$$\bar{c}_p = a \left(\frac{T}{1000} \right) + \frac{bT}{2} \left(\frac{T}{1000} \right)^2 + \frac{cT}{3} \left(\frac{T}{1000} \right)^3 \quad \left[\frac{J}{mol-K} \right]$$

Perform calculations on spreadsheet to solve for required parameters.

(f) Plot of specific heat of H_2O , O_2 and H_2 as a function of temperature



(e) Plot of total enthalpy as a function of temperature (Bonus +5 Points)

