Name: Veronica Loomis

SPA

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

$\delta Q = 0$

$H_2 = H_1$

Find: a) Adiabatic flame temp, T_c

b) coefficient of the products, a

c) Molecular weight of products, M

d) The gamma of the products

e) Characteristic velocity of the products, c^*

f) Plot specific heat of water as function of temp

g) BONUS: Plot total enthalpy as function of temperature

Schematic: ∅

Assumptions: Adiabatic combustion

No dissociation

Heat of formation from Table 5.1

Specific heat fits Table 5.3

P = 1 atm

Reactants are 298 K

Equations:

$$h_{A_i} = \int_{T^0}^{T} C_{PA_i}\, dT + h^{\circ}_{A_i}$$

$$M = \frac{1}{\sum_{i=1}^{N} Y_i / M_i}$$

$$\gamma_{mix} = \frac{C_{Pmix}}{C_{Pmix} - R_{mix,u}}$$

$$c^* = \sqrt{\frac{R_u T_c}{\gamma M}}\left[2/(\gamma+1)\right]^{-(\gamma+1)/2(\gamma-1)}$$

Analysis:

a) $$2\left[h^{\circ} + \int_{298}^{T_c} C_p dT\right]_{H_2O} = 2\left[h^{\circ} + \int_{298}^{298} C_p dT\right]_{H_2} + \left[h^{\circ} + \int_{298}^{298} C_p dT\right]_{O_2}$$

$$h^{\circ}_{H_2O} = -57.7979 \text{ kcal/mole}$$

$$C_{P\,H_2O} = 29.182 + 14.503\,(T/1000) - 2.0235\,(T/1000)^2 \quad \text{J/gmole K}$$

$$\int C_{P\,H_2O} = 29.182\,T + \frac{14.503}{2} T(T/1000) - \frac{2.0235}{3} T\,(T/1000)^2$$

$$2\left\{-57.7979 \frac{\text{kcal}}{\text{mole}} \times \frac{4184 \text{ J}}{\text{kcal}} + \left[29.182\,T + \frac{14.503}{2} T(T/1000) - \frac{2.0235}{3} T(T/1000)^2 \ \text{J/gmole K}\right]_{298}^{T_c}\right\} = 0$$

calculated using MATLAB

$$\boxed{T_c = 5163.9956 \text{ K}}$$

b) Since it's complete combustion, $\boxed{a = 2}$

c) $2H_2O$

H: $4(1.01) = 4.04$ g/gmol

O: $2(16) = 32$ g/gmol

$$\boxed{M = 36.04 \text{ g/gmol}}$$

d) $c_p = 29.182 + 14.503\left(\frac{5163.9956}{1000}\right) - 2.0235\left(\frac{5163.9956}{1000}\right)^2$

$c_p = 50.115$ J/gmol K

$R_u = 8.317 \frac{Nm}{gmol\,K}$

$$\gamma = \frac{50.115 \frac{Nm}{gmol\,K}}{50.115 - 8.317 \frac{Nm}{gmol\,K}}$$

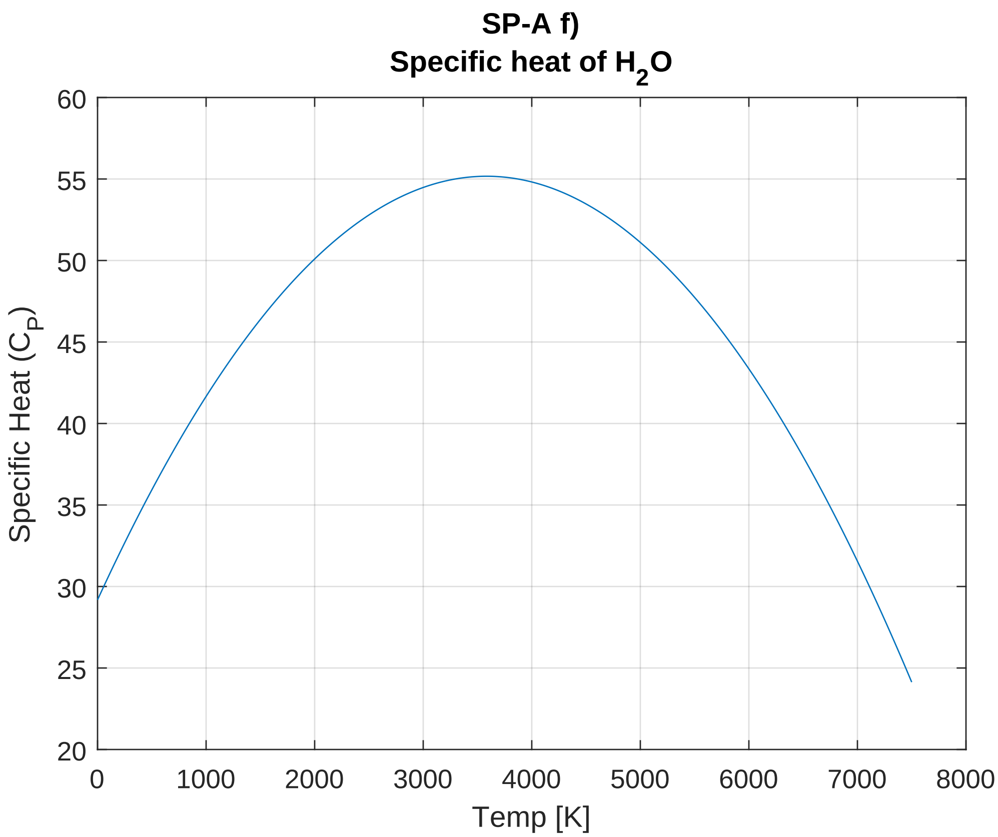
$$\boxed{\gamma = 1.194}$$

e) $c^* = \sqrt{\frac{R_u T_c}{\gamma M}}\,(2/(\gamma+1))^{-(\gamma+1)/2(\gamma-1)}$

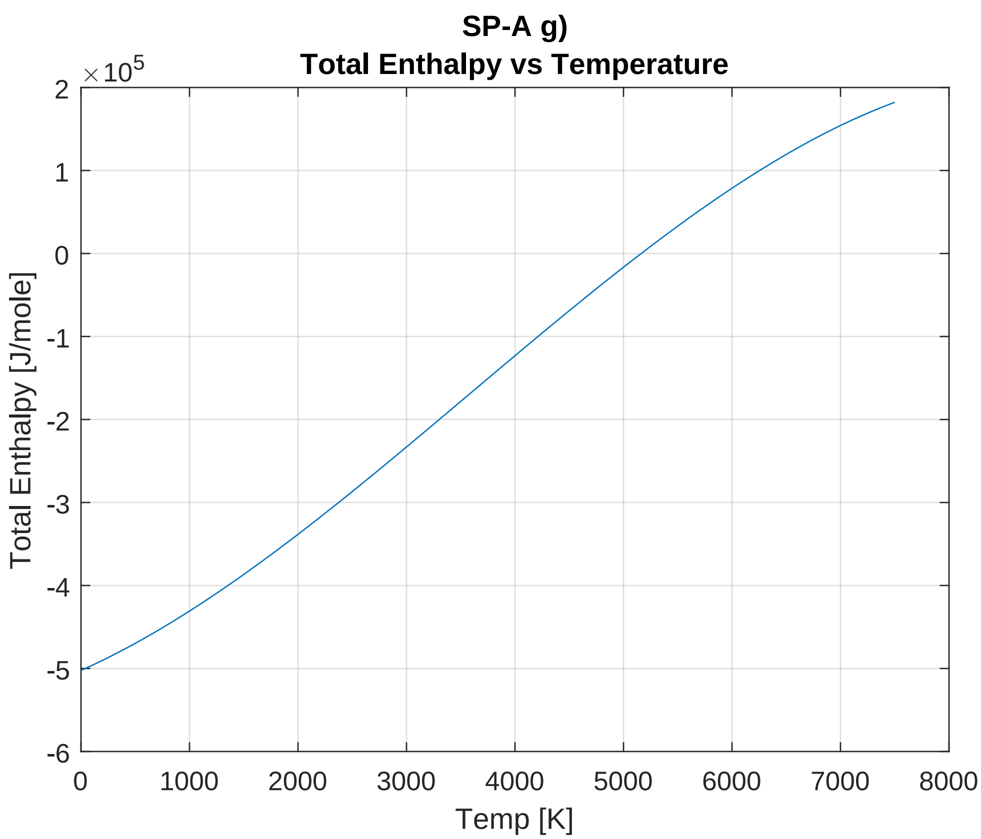
$$c^* = \sqrt{\frac{(8.314)\frac{Nm}{gmol\,K}(5163.9956)\,K}{(1.194)(36.04)\,g/gmol} \times 1000\ g/kg}\;(2/(1.194+1))^{-2.194/2(0.194)}$$

$$\frac{Nm}{gmol}\;\frac{gmol}{g} = kg\frac{m}{s^2}\;\frac{m}{g} \times \frac{1000g}{kg}$$

$$\boxed{c^* = 1686 \text{ m/s}}$$



SP-A f)
Specific heat of H_2O
Specific Heat (C_P)
Temp [K]
60
55
50
45
40
35
30
25
20
0
1000
2000
3000
4000
5000
6000
7000
8000


SP-A g)
Total Enthalpy vs Temperature
×10^5
2
1
0
-1
-2
-3
-4
-5
-6
0
1000
2000
3000
4000
5000
6000
7000
8000
Temp [K]
Total Enthalpy [J/mole]

Name: Veronica Loomis

SP B

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

Find: a) Adiabatic flame temp, T_c

b) Coefficient of products, a

c) Molecular weight of products, M

d) Gamma of the products

e) Characteristic velocity of the products, c^*

f) Plot of specific heat of water, O_2, and H_2 as function of temp

g) Bonus: Plot of total enthalpy as function of temp

Schematic: Ø

Assumptions: Adiabatic combustion

No dissociation

Heat of formation from table 5.1

Specific heats from table 5.3

P = 1 atm

Reactant temp = 298 K

One dissociation reaction

equilibrium constants from Purdue

Equations:

$$h_{A_i} = \int_{T^0}^{T} c_{PA_i}\, dT + h^0_{A_i}$$

$$\gamma_{mix} = \frac{c_{p\,mix}}{c_{p\,mix} - R_u}$$

$$c^* = \sqrt{\frac{R_u T_c}{\gamma M}}\left[2/(\gamma+1)\right]^{-(\gamma+1)/2(\gamma-1)}$$

$$K_p = a(6-a)^{1/2}/(2-a)^{3/2}$$

Analysis:

a)

$$a\left[-57800 \tfrac{cal}{mol} \times 4.184 \tfrac{J}{cal}\right] + \left[29.182T + \frac{14.503}{2}T(T/1000) - \frac{2.0235}{3}T(T/1000)^2\right]_{298}^{T_c}$$
$$+ (2-a)\left[26.896T + \frac{4.35011}{2}T(T/1000) - \frac{0.32674}{3}T(T/1000)^2\right]_{298}^{T_c}$$
$$+ \frac{2-a}{2}\left[28.186T + \frac{6.3011}{2}T(T/1000) - \frac{0.74986}{3}T(T/1000)^2\right]_{298}^{T_c} = 0$$

Solve in MATLAB

$\boxed{T_c = 3500\,K}$

b) $K_p = 10^{\wedge}\, BT^3 + CT^2 + DT + E$

B = -1.8559e-10

C = 2.3375 e -6

D = -1.05e -2

E = 1.6715 e1

$K_p = 4.3874$

$K_p = \frac{a(6-a)^{1/2}}{(2-a)^{3/2}}$

$\boxed{a = 1.2666}$

c) $2H_2 + O_2 \rightarrow 1.266\,H_2O + 0.367\,O_2 + 0.734\,H_2$

$M = 1.266(2.02 + 16) + 0.367(32) + 0.734(2.02)$ g/gmol

$M = 22.813 + 11.744 + 1.48268$ g/gmol

$\boxed{M = 36.04 \text{ g/gmol}}$

d) $C_p =$ oh boy

$C_{p\,H_2O} @ 3500K = 29.182 + 14.503(3500/1000) - 2.0235(3500/1000)^2 =$

$C_{p\,H_2} @ 3500K = 26.896 + 4.3501(3500/1000) - 0.32674(3500/1000)^2 =$

$C_{p\,O_2} @ 3500K = 28.186 + 6.3011(3500/1000) - 0.74986(3500/1000)^2 =$

$C_p = 134.3271$ J/gmol K

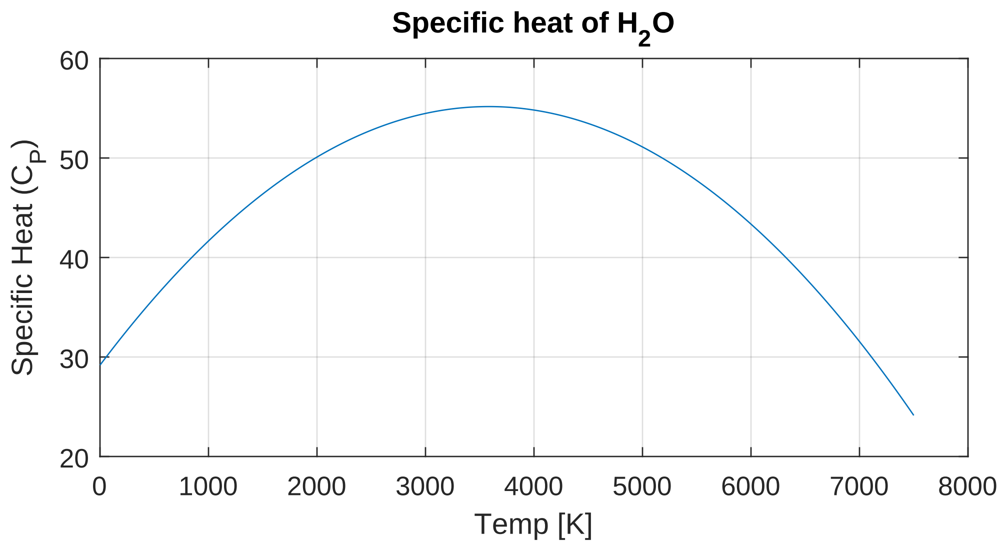
$$\gamma = \frac{C_p}{C_p - R_u}$$

$$\gamma = \frac{134.3271}{134.3271 - 8.317}$$

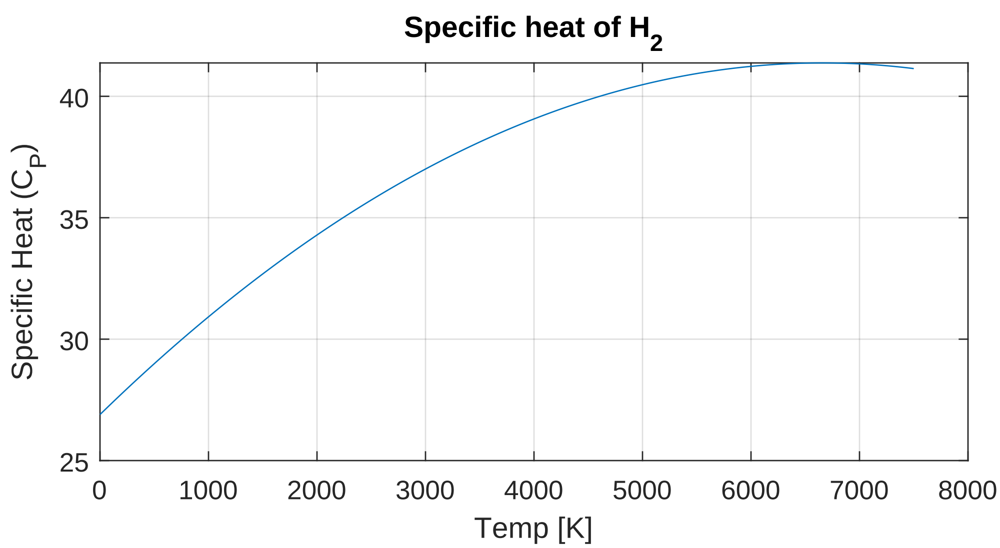
$\boxed{\gamma = 1.066}$

e) $$c^* = \sqrt{\frac{8.317 \frac{Nm}{gmol\,K} \times 3500\,K \times 1000\,g/kg}{1.066 \times 36.04\,g/gmol}\left[2/2.066\right]^{-2.066/2(0.066)}}$$

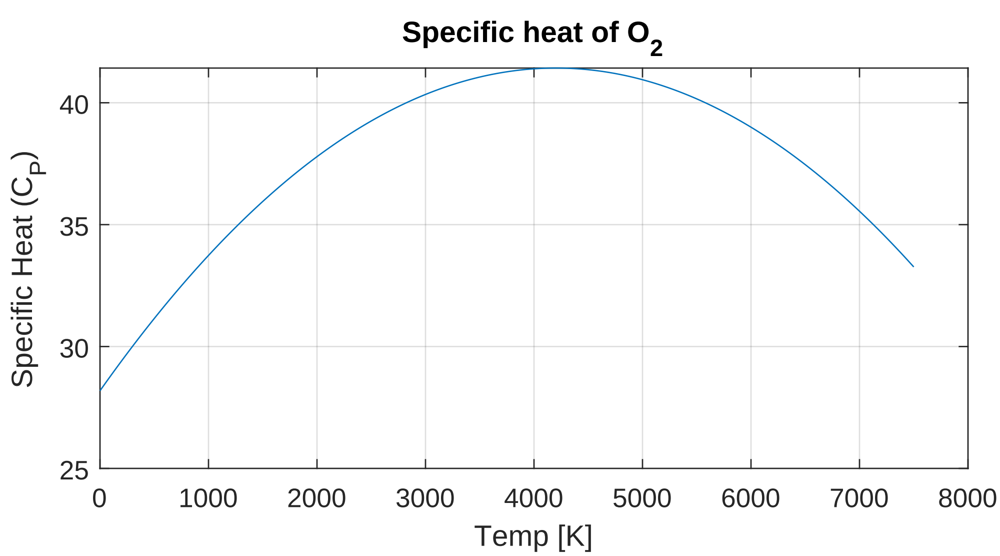
$\boxed{c^* = 1446.6 \text{ m/s}}$



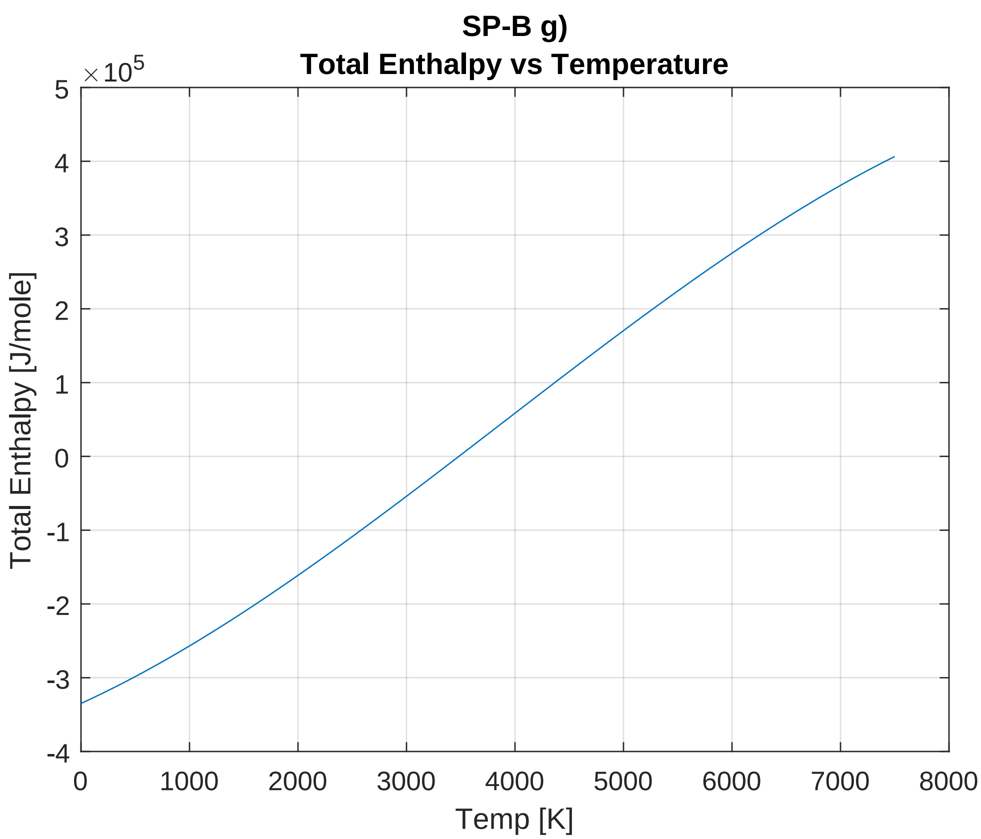
Specific heat of H_2O
Specific Heat (C_P)
Temp [K]
60
50
40
30
20
0
1000
2000
3000
4000
5000
6000
7000
8000



Specific heat of H_2
Specific Heat (C_P)
Temp [K]
40
35
30
25
0
1000
2000
3000
4000
5000
6000
7000
8000



Specific heat of O_2
Specific Heat (C_P)
Temp [K]
40
35
30
25
0
1000
2000
3000
4000
5000
6000
7000
8000


SP-B g)
Total Enthalpy vs Temperature
×10^5
5
4
3
2
1
0
-1
-2
-3
-4
Total Enthalpy [J/mole]
0
1000
2000
3000
4000
5000
6000
7000
8000
Temp [K]

Name: Veronica Loomis__________

03HW-A Summary One-Page Cover Sheet

03HW-A-SP Summary of Results Omit Problem 5.4 and 5.16

Final Chemical Equation for SP03-A_A

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

Final Chemical Equation for SP03-A_B

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

Result	SP03-A_A	SP03-A_B	Comment on Reasons for Any Differences
Adiabatic Flame Temperature, [*K*]	5163.9956	3500	Since SP-A is complete combustion, it makes sense that its flame temperature is much larger than the temperature from incomplete combustion
"*a*" for H_2O [*kgmole*]	2	1.2666	For SP-B being incomplete, the full H_2O is not formed so it is less than 2
"*b*" for O_2 [*kgmole*]	0	0.367	SP-A is complete combustion, so the other components are zero
"*c*" for H_2 [*kgmole*]	0	0.734	SP-A is complete combustion, so the other components are zero
$\mathcal{M}$ [*kg/kgmole*]	36.04	36.04	The molar mass is the same since we start with the same reactants
*c** [*m/s*]	1686	1446.6	A higher flame temperature gives a higher characteristic velocity

Copy of the "Reflect" Section of Your Literature Review (Gordon and McBride)

This article is convenient source for many equations and realizing where the enthalpy calculations are derived from. It includes not only the equations themselves, but also describes the special cases in which they can be edited.

Summarize

Reference Document Examined:	Gordon and McBride, “Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouget Detonations”
Reviewer:	Veronica Loomis
Source of Document:	canvas
Date of Review:	February 7, 2023
Electronic File Name:	**Ref_NASA_SP273.pdf**

Summary of Paper:

This article lists a bunch of useful equations for things such as enthalpies; continuity, momentum, and energy conservation equations; flow velocities; forces; specific impulse; and characteristic velocity.

B. Assess:

Important Facts from Document:

1. In general, the specific heat (H_T^O) does NOT equal the flame specific heat ($\left(H_f^O\right)_T$) at a temperature other than 298.15K.
2. It is assumed that there is one-dimensional form of the continuity, energy and momentum equations.
3. It is assumed that there is zero velocity in the combustion chamber.
4. It is assumed that the combustion is complete and adiabatic.
5. It is assumed that there are zero temperature and velocity lags between condensed and gaseous species.

Key Figure from Document:

n/a

Important Relationships among Parameters Described in the Paper:

1. For reference elements, $\left(\Delta H_f^O\right)_{298.15} = H_{298.15}^O = 0.$
2. Cryogenic liquids assigned enthalpies are given at their boiling points and are usually obtained by subtracting the following quantities from the heat of formation of the gas phase at 298.15 K: sensible heat between 298.15 K and the boiling point, difference in enthalpy between ideal gas and real gas at the boiling point, and heat of vaporization at the boiling point.

C. Reflect

This article is convenient source for many equations and realizing where the enthalpy calculations are derived from. It includes not only the equations themselves, but also describes the special cases in which they can be edited.

Table of Contents

SP-A e)

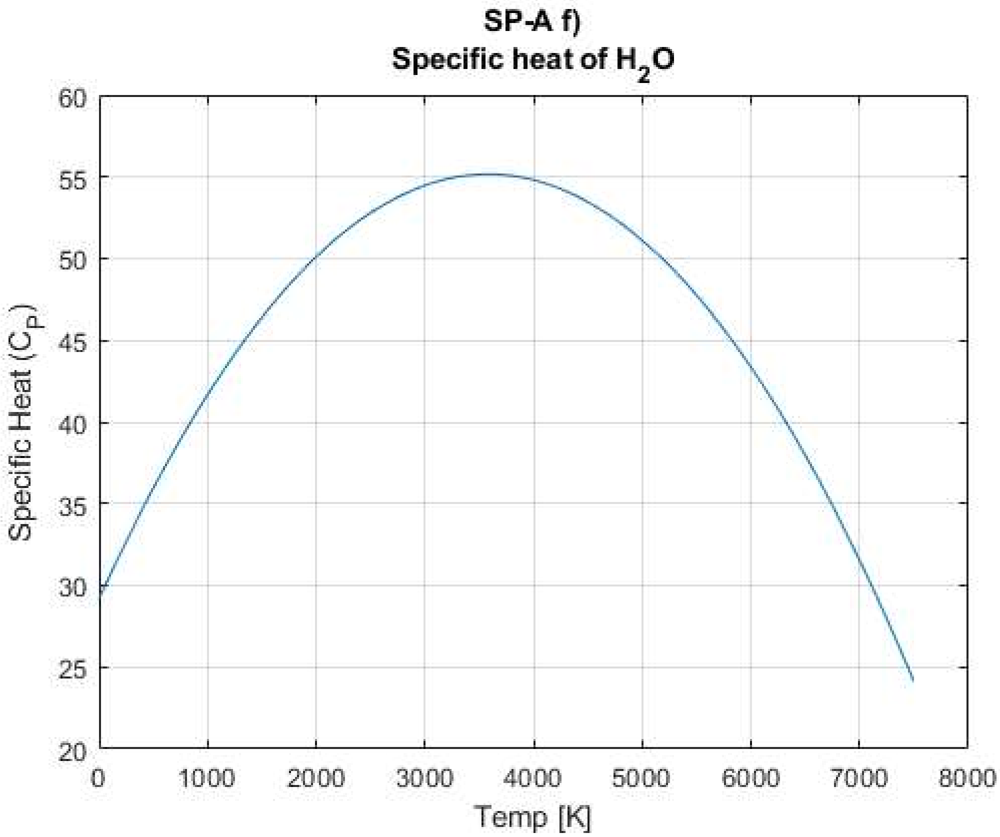
Characteristic velocity

```
Ru = 8.314;
Tc = 5163.9956;
gamma = 1.194;
molarMass = 36.04;

cStar = sqrt(1000*Ru*Tc/(gamma*molarMass)) * (2/(gamma+1))^(-(gamma+1)/
(2*(gamma-1)));
```

SP-A f)

Plot Specific Heat of water as a function of temperature

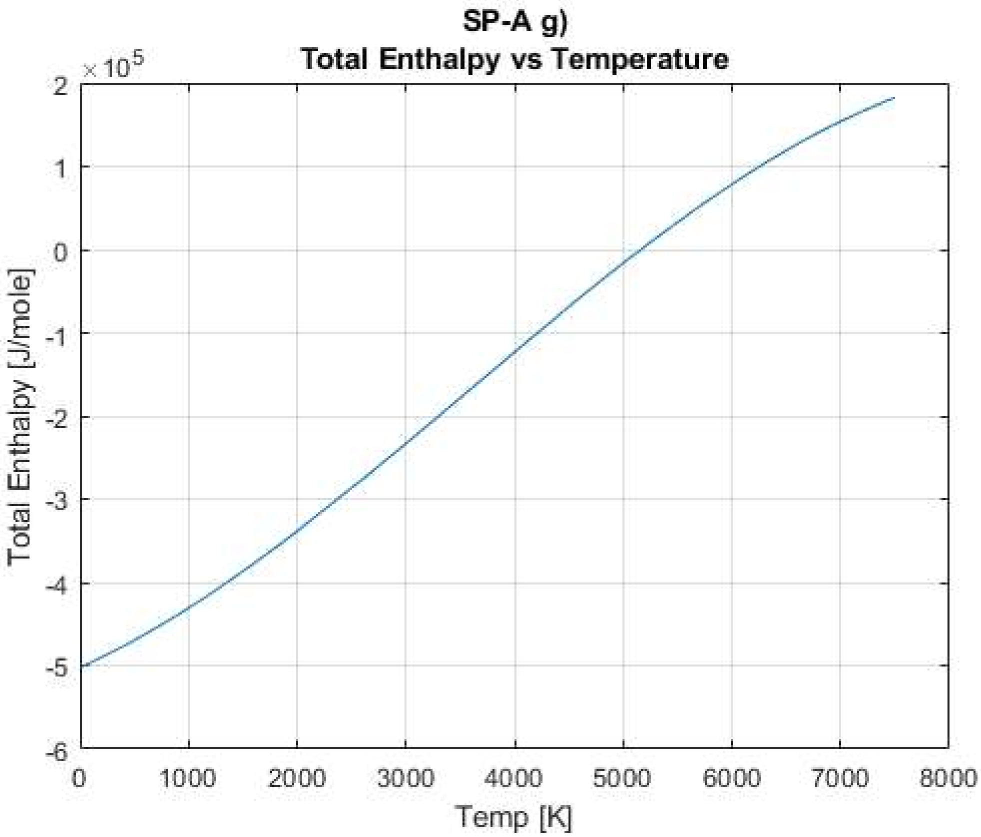
```
T = linspace(0,7500,1000);
cP = 29.182 + 14.503*(T/1000) - 2.0235*(T/1000).^2;

figure(1)
plot(T,cP)
grid on
title({'SP-A f)','Specific heat of H_2O'})
xlabel('Temp [K]')
ylabel('Specific Heat (C_P)')
```



SP-A g)

Plot total enthalpy as a function of temperature

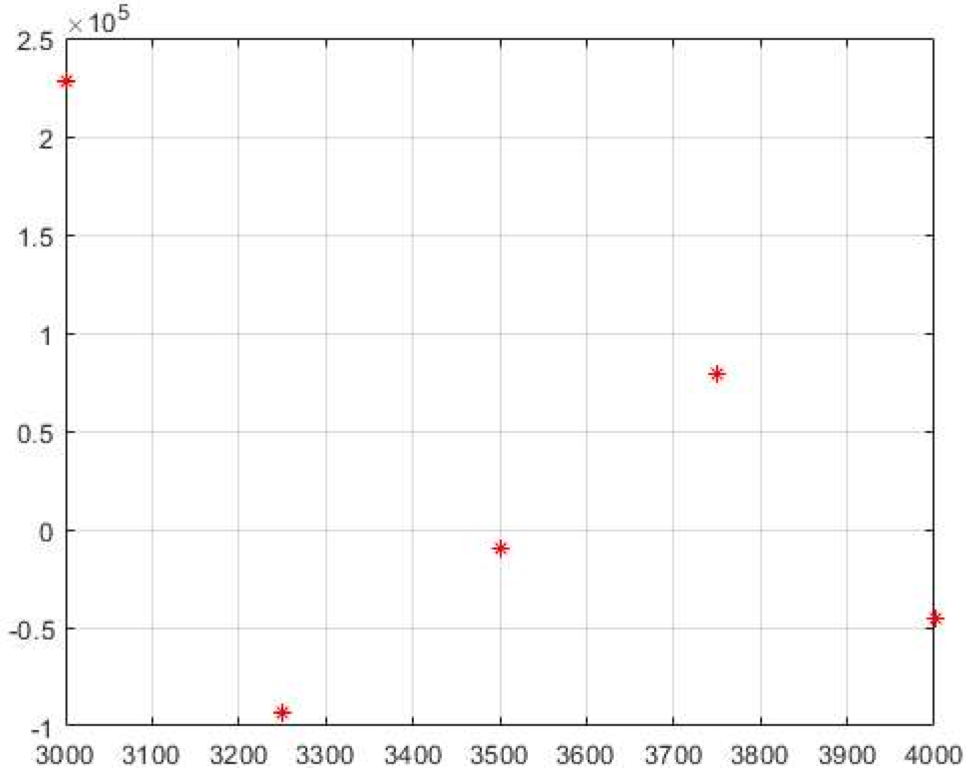
```
T = linspace(0,7500,1000);
enthalpyA = 2*(-57.7979*4184 + 29.182*T + (14.503/2)*T.*(T/1000) -
 (2.0235/3)*T.*(T/1000).^2 - (29.182*298 + (14.503/2)*298*(298/1000) -
 (2.0235/3)*298*(298/1000).^2));

figure(2)
plot(T, enthalpyA)
grid on
title({'SP-A g)','Total Enthalpy vs Temperature'})
xlabel('Temp [K]')
ylabel('Total Enthalpy [J/mole]')
```



SP-B a)

guess T use that to get Kp use that to find a plug in to equation and see how it looks

```
Ts = [3000, 3250, 3500, 3750, 4000];
kp = [0.21, 9.5786, 4.9295, 2.7498, 16.623];
a =  [0.20914, 1.51728, 1.309, 1.0852, 1.65];


for i=1:length(Ts)
    enthalpyB(i) = a(i)*((-57800*4.184) + (29.182*Ts(i) +
 (14.503/2)*Ts(i)*(Ts(i)/1000) - (2.0235/3)*Ts(i)*(Ts(i)/1000)^2) -
 ((29.182*298 + (14.503/2)*298*(298/1000) - (2.0235/3)*298*(298/1000)^2 )))...
        + (2 - a(i))*(26.896*Ts(i) + (4.35011/2)*Ts(i)*(Ts(i)/1000) -
 (0.32674/3)*Ts(i)*(Ts(i)/1000)^2) - (26.896*298 + (4.35011/2)*298*(298/1000)
 - (0.32674/3)*298*(298/1000)^2)...
        + ((2-a(i))/2)*(28.186*Ts(i) + (6.3011/2)*Ts(i)*(Ts(i)/1000) -
 (0.74986/3)*Ts(i)*(Ts(i)/1000)^2) - (28.186*298 + (6.3011/2)*298*(298/1000) -
 (0.74986/3)*298*(298/1000)^2);
end

plot(Ts,enthalpyB,'r*')
grid on
```



SP-B b)

```
B = -1.8559E-10;
C = 2.3375E-06;
D = -1.0500E-02;
E = 1.6715E+01;

T = 3500;

kp = B*T^3 + C*T^2 + D*T + E;
```

SP-B d)

```
cph2o = 29.182 + 14.503*(3500/1000) - 2.0235*(3500/1000)^2;
cph2 = 26.896 + 4.350*(3500/1000) - 0.32674*(3500/1000)^2;
cpo2 = 28.186 + 6.3011*(3500/1000) - 0.74986*(3500/1000)^2;

cp = cph2o + cph2 + cpo2;
```

SP-B e)

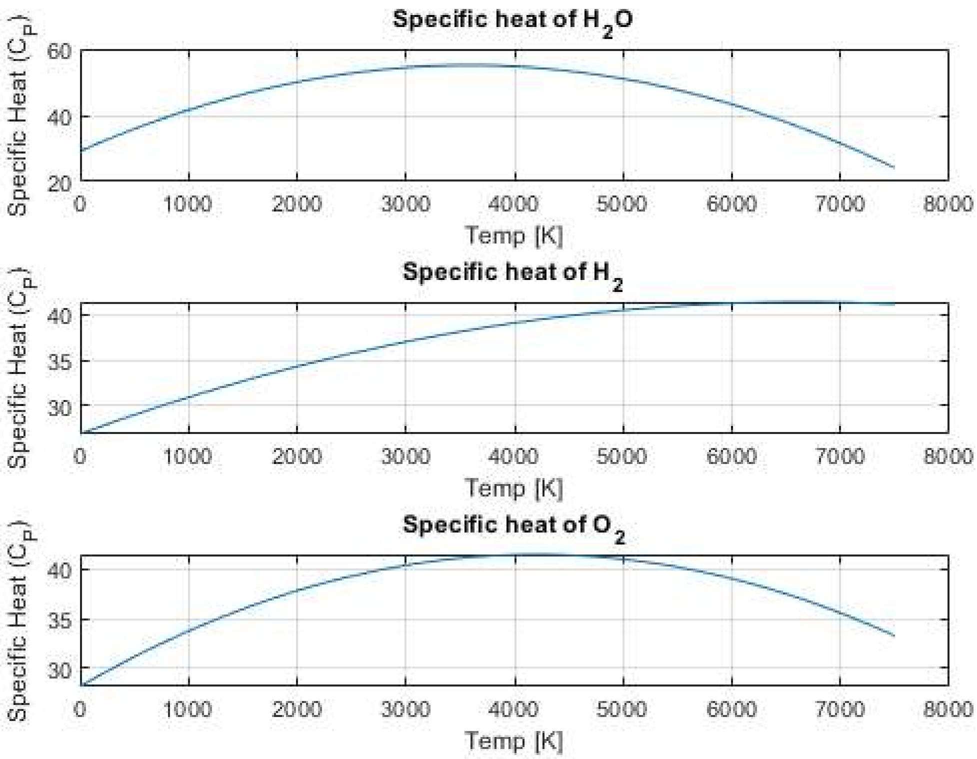
```
Ru = 8.314;
Tc = 3500;
gamma = 1.066;
```

```
molarMass = 36.04;

cStar = sqrt(1000*Ru*Tc/(gamma*molarMass)) * (2/(gamma+1))^(-(gamma+1)/
(2*(gamma-1)));
```

SP-B f)

Plot Specific Heat of water as a function of temperature

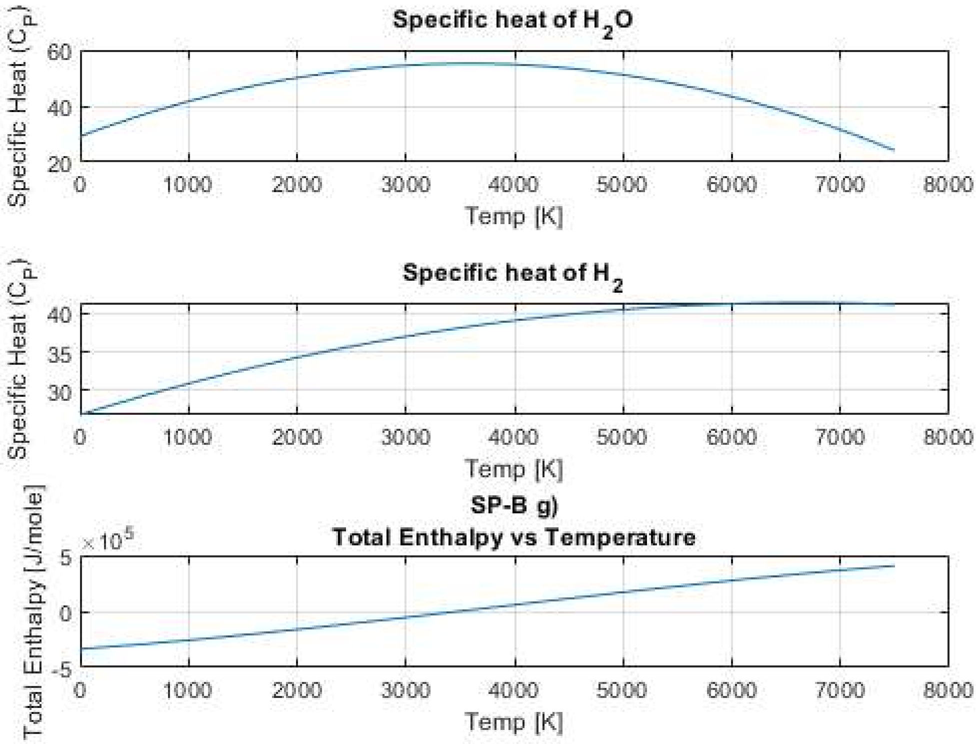
```
T = linspace(0,7500,1000);
cph2o = 29.182 + 14.503*(T/1000) - 2.0235*(T/1000).^2;
cph2 = 26.896 + 4.350*(T/1000) - 0.32674*(T/1000).^2;
cpo2 = 28.186 + 6.3011*(T/1000) - 0.74986*(T/1000).^2;

figure(3)
subplot(3,1,1)
plot(T,cph2o)
grid on
title('Specific heat of H_2O')
xlabel('Temp [K]')
ylabel('Specific Heat (C_P)')
subplot(3,1,2)
plot(T,cph2)
grid on
title('Specific heat of H_2')
xlabel('Temp [K]')
ylabel('Specific Heat (C_P)')
subplot(3,1,3)
plot(T,cpo2)
grid on
title('Specific heat of O_2')
xlabel('Temp [K]')
ylabel('Specific Heat (C_P)')
```



SP-A g)

Plot total enthalpy as a function of temperature

```
Ts = linspace(0,7500,1000);
a = 1.266;
enthalpy = a*((-57800*4.184) + (29.182*Ts + (14.503/2)*Ts.*(Ts/1000) -
 (2.0235/3)*Ts.*(Ts/1000).^2) - ((29.182*298 + (14.503/2)*298*(298/1000) -
 (2.0235/3)*298*(298/1000)^2 )))...
        + (2 - a)*(26.896*Ts + (4.35011/2)*Ts.*(Ts/1000) -
 (0.32674/3)*Ts.*(Ts/1000).^2) - (26.896*298 + (4.35011/2)*298*(298/1000) -
 (0.32674/3)*298*(298/1000)^2)...
        + ((2-a)/2)*(28.186*Ts + (6.3011/2)*Ts.*(Ts/1000) -
 (0.74986/3)*Ts.*(Ts/1000).^2) - (28.186*298 + (6.3011/2)*298*(298/1000) -
 (0.74986/3)*298*(298/1000)^2);
plot(T, enthalpy)
grid on
title({'SP-B g)','Total Enthalpy vs Temperature'})
xlabel('Temp [K]')
ylabel('Total Enthalpy [J/mole]')
```



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