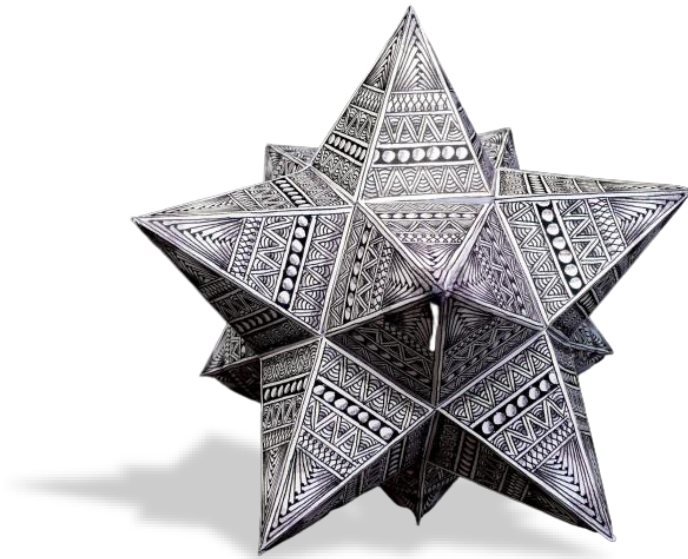# AAE339: Aerospace Propulsion

HW4: Propulsion Thermochemistry

Dr. Anderson

Tomoki Koike

February 12, 2020

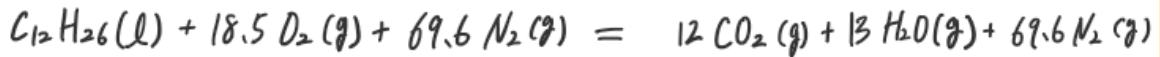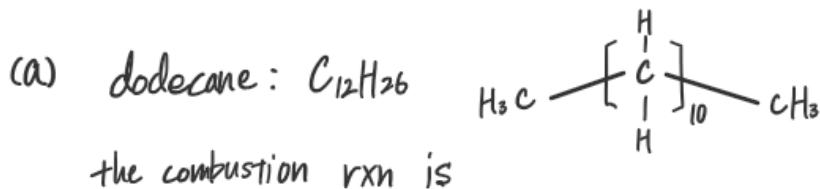## Problem 1. Basic properties of reacting flows

Write balanced chemical equations for the following reactions in terms of major stable species. Calculate the molecular weight of the product mixture. For a pressure of 0.5 MPa, calculate the partial pressure of each species in the product stream, ie on the right side of the equation.

a)   dodecane and air; FAR = 0.03
b)   hydrogen and oxygen; $\phi = 1.33$
c)   oxygen and ethanol (C_2H_5OH); O/F = 4.0

In each case, first write out the reaction for stoichiometric conditions ($\phi = 1$), and define the stoichiometric coefficient for the reactants and products.

$$M_{O_2} = 32 \ \frac{g}{mol} \qquad M_{CO_2} = 44 \ \frac{g}{mol} \qquad M_{H_2O} = 18 \ \frac{g}{mol}$$

$$M_{N_2} = 28 \ \frac{g}{mol}$$

(a)   dodecane: $C_{12}H_{26}$

$$H_3C \underbrace{\left[\begin{array}{c} H \\ | \\ C \\ | \\ H \end{array} \right]_{10}} CH_3$$

the combustion rxn is

$$\boxed{C_{12}H_{26}(l) + 18.5 \ O_2(g) + 69.6 \ N_2(g) = 12 \ CO_2(g) + 13 \ H_2O(g) + 69.6 \ N_2(g)}$$

stoichiometric

$$FAR := \text{fuel-air ratio} = 0.03$$

which means

$$\left(\frac{f}{a}\right)_{op} = \frac{\dot{m}_f}{\dot{m}_{air}} = 0.03$$

in stoichiometric condition

$C_{12}H_{26}$: $1 \ mol \times 170 \ \frac{g}{mol} = 170 \ g$ $\qquad O_2 : 18.5 \ mol \times 36 \ \frac{g}{mol} = 666 \ g$

N_2 : $69.6 \ mol \times 28 \ \frac{g}{mol} = 1949 \ g$ $\qquad CO_2 : 12 \ mol \times 44 \ \frac{g}{mol} = 528 \ g$

H_2O : $13 \ mol \times 18 \ \frac{g}{mol} = 234 \ g$

2

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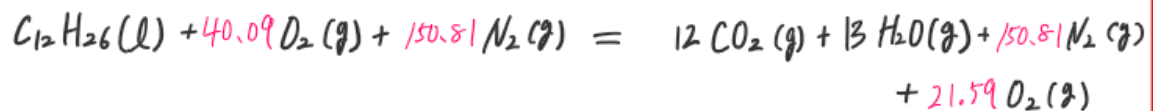
then $\left(\dfrac{f}{a}\right)_{stoich} = \dfrac{170\ g}{666g + 1949\ g} = 0.065$

thus $\varphi = \dfrac{(f/a)_{op}}{(f/a)_{stoich}} = \dfrac{0.03}{0.065} = 0.4615$

from φ we know there is

$\dfrac{1}{0.4615} = 2.1668$ times more air than the stoichiometric condition

thus, the chemical rxn becomes

$$C_{12}H_{26}(l) + 40.09\ O_2(g) + 150.81\ N_2(g) = 12\ CO_2(g) + 13\ H_2O(g) + 150.81\ N_2(g) + 21.59\ O_2(g)$$

thus, $MW_{product} = \dfrac{(12 \times 14 + 13 \times 18 + 150.81 \times 28 + 21.59 \times 32)\ g}{(12 + 13 + 150.81 + 21.59)\ mol}$

$= \boxed{26.93\ \dfrac{g}{mol}}$

now if the total pressure is $25 MPa = P_{tot}$

the total pressure is dependent on the total moles of the products

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$$\frac{n_{Tot} RT}{V} = P_{Tot}$$

thus,
$$P_{CO_2} = \frac{n_{CO_2} RT}{V} = \frac{n_{CO_2}}{n_{Tot}} \frac{n_{Tot} RT}{V}$$

$$P_{CO_2} = \left(\frac{12}{197.4}\right) 0.5 MPa = 0.0304 \ MPa$$

similarly

$$P_{H_2O} = \left(\frac{13}{197.4}\right) 0.5 MPa = 0.0329 \ MPa$$

$$P_{N_2} = \left(\frac{150.81}{197.4}\right) 0.5 MPa = 0.3820 MPa$$

$$P_{O_2} = \left(\frac{21.59}{197.4}\right) 0.5 MPa = 0.0547 MPa$$

(b) Hydrogen & Oxygen $\varphi = 1.33$
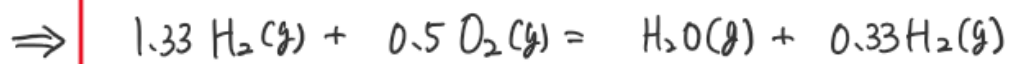
$$H_2 (g) + 0.5 \ O_2 (g) = H_2O (g)$$
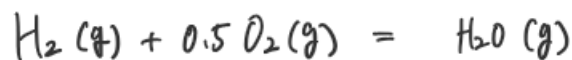
stoichiometric

now because $\varphi = 1.33$ we know that there is

$\varphi = 1.33$ times more fuel/hydrogen than oxygen

wrt the stoichiometric condition above

therefore the balanced equation becomes

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$$\Rightarrow \boxed{1.33\,H_2(g) + 0.5\,O_2(g) = H_2O(g) + 0.33\,H_2(g)}$$

$$\therefore \quad MW_{product} = \frac{(18 + 0.33 \times 2)g}{(1 + 0.33)mol} = \boxed{14.03\,g/mol}$$

then

$$\boxed{\begin{array}{l} P_{H_2O} = \left(\frac{1}{1.33}\right)0.5\,MPa = 0.3759\,MPa \\[2mm] P_{H_2} = \left(\frac{0.33}{1.33}\right)0.5\,MPa = 0.1241\,MPa \end{array}}$$

(C) C_2H_5OH ethanol and O_2 oxygen $(O/F)_{op} = 4.0$

$$\boxed{C_2H_5OH\,(\ell) + 3.5\,O_2(g) = 2\,CO_2(g) + 3\,H_2O(g)}$$
stoichiometric

here

$$\left(\frac{O}{F}\right)_{stoich} = \frac{3.5 \times 32\,g/mol}{1 \times 46\,g/mol} = 2.4348$$

now

$$\varphi = \frac{(O/F)_{stoich}}{(O/F)_{op}} = \frac{2.4348}{4.0} = 0.6087$$

from this we know that there is $\frac{1}{0.6087} \approx 1.6428$

times more oxygen than ethanol wrt stoichiometric

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condition, Thus, the balanced equation becomes

$$C_2H_5OH(\ell) + 5.7498\, O_2(g) = 2\, CO_2(g) + 3\, H_2O(g) + 2.2498\, O_2(g)$$
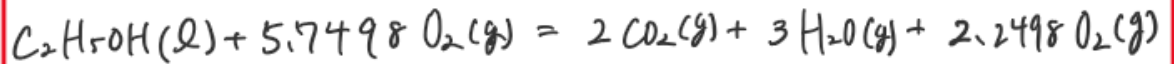
now

$$MW_{product} = \frac{(2\times44 + 3\times18 + 2.2498\times32)\, g}{(2 + 3 + 2.2498)\, mol} = 29.52\, \tfrac{g}{mol}$$

finally,

$$P_{CO_2} = \left(\frac{2}{7.2498}\right) 0.5\, MPa = 0.1379\, MPa$$

$$P_{H_2O} = \left(\frac{3}{7.2498}\right) 0.5\, MPa = 0.2069\, MPa$$

$$P_{O_2} = \left(\frac{2.2498}{7.2498}\right) 0.5\, MPa = 0.1552\, MPa$$

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Problem 2. Heat of reaction and adiabatic flame temperature of a simple reaction

Propane ($\Delta h_f^0 = -104 \, kJ/mole$) and air react at 298K and 1 atm and at $\phi = 0.8$. Remember to start by writing the chemical equation for this reaction at $\phi = 1.0$, and then adjust the reaction to the given equivalence ratio. Assume the product stream comprises only H_2O, CO_2, and what is left over from the excess reactants. Calculate the ==heat of reaction==, in terms of ==kJ/mole of propane.== Then calculate the ==adiabatic flame temperature at $\phi = 0.8$.== ==Consider the temperature dependency of heat capacity in your== ==calculation by using the table of $c_p(T)$ in Appendix II of your textbook.== To balance the heat of reaction with the temperature rise of the products, $-\Delta H_{rxn} = \sum_{products,i} \int_{T^0}^{T_{ad}} n_i c_{p,i} dT$, use one of two methods. The first uses an iterative approach - guess a value for the AFT, and then check the energy balance by calculating the right hand side term. Iterate until successive estimates of the temperatures converge within 150K. Alternatively, construct a table of the RHS term as a function of T, and determine T_{ad} by inspection of the table. Next, use CEA (https://cearun.grc.nasa.gov/) to calculate the flame temperature and compare it to your final estimate. Compare the composition of the combustion products from CEA and your written chemical reaction at $\phi = 0.8$ in terms of their mole fractions.

(i) Chemical eqn.

propane C_3H_8 : $CH_3-CH_2-CH_3$ $M_{C_3H_8} = 44 \, g/mol$
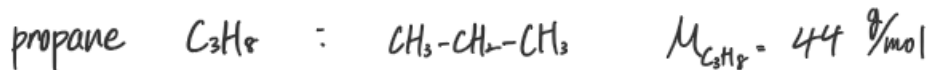
the balanced chemical rxn becomes (air $N_2: 79\%$ $O_2: 21\%$)

$\therefore \quad 5 \div 21 \times 79 = 18.81$

$$C_3H_8 (g) + 5 O_2(g) + 18.81 \, N_2(g) = 3 CO_2(g) + 4 H_2O(g) + 18.81 \, N_2(g)$$
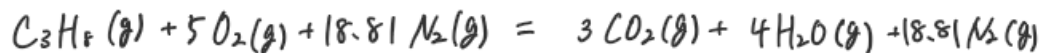
stoichiometric

now since $\phi = 0.8$

we know that $\frac{1}{0.8} = 1.25$ times more O_2 exists than wrt stoichiometric conditions

$5 \times 1.25 = 6.25$, $18.81 \times 1.25 = 23.513$

than the balanced rxn equation becomes

$$C_3H_8(g) + 6.25 \, O_2(g) + 23.513 \, N_2(g) = 3 CO_2(g) + 4 H_2O(g) + 23.513 N_2(g) + 1.25 O_2(g)$$

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(ii) heat of rxn.

the heat of formation for each reactants & products are
from the lecture slide

C_3H_8 : -103.8 kJ/mol   From: https://webbook.nist.gov/cgi/cbook.cgi?ID=C74986&Mask=1

N_2 : 0

O_2 : 0

CO_2 : -393.522 kJ/mol

H_2O : -241.826 kJ/mol

$$\therefore \Delta H^0 = \left[3 \times (-393.522 \text{ kJ/mol}) + 4 \times (-241.826 \text{ kJ/mol}) \right] - \left[-103.8 \text{ kJ/mol} \right]$$

$$= \boxed{-2044.07 \text{ kJ/mol} \quad \text{propane}}$$

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(iii) Adiabatic temperature

since C_p is a func of θ (on the slides)

$$N_2: \bar{C}_{p0} = 39.060 - 512.79\,\theta^{-1.5} + 1072.7\,\theta^{-2} - 820.40\,\theta^{-3}$$

$$O_2: \bar{C}_{p0} = 37.432 + 0.020102\,\theta^{1.5} - 178.57\,\theta^{-1.5} + 236.88\,\theta^{-2}$$

$$CO_2: \bar{C}_{p0} = -3.7357 + 30.529\,\theta^{0.5} - 4.1034\,\theta + 0.024198\,\theta^{2}$$

$$H_2O: \bar{C}_{p0} = 143.05 - 183.54\,\theta^{0.25} + 82.751\,\theta^{0.5} - 3.6989\,\theta$$

now from

$$-\Delta H_{rxn} = \sum_{products,\,i} \int_{T_{ref}}^{T_{ad}} n_i C_{p,i}\, dT$$

$$\begin{cases} \theta = \dfrac{T}{100} \iff d\theta = \dfrac{dT}{100} \iff dT = 100\,d\theta \\[2mm] T: T_{ref} \to T_{ad} \iff \theta: \dfrac{T_{ref}}{100} = \theta_{ref} \to \dfrac{T_{ad}}{100} = \theta_{ad} \end{cases}$$

$$-(-2044.07 \; {}^{kJ}\!/_{mol}) = \sum_{product,\,i} \int_{\theta_{ref}}^{\theta_{ad}} 100\, n_i\, C_{p,i}\, d\theta \quad \left(\theta: {}^{kJ}\!/_{kmol} = {}^{J}\!/_{mol}\right)$$

$$\Downarrow$$

$$* \; \left(2044.07 \; {}^{kJ}\!/_{mol}\right) \cdot \frac{1000\,J}{1\,kJ} = 2,044,070$$

(matlab code is in appendix)

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solving by using optimization method in MATLAB by minimizing the function below (to zero)

$$abs \left[\sum_{products,i} \int_{T_{ref}}^{T_{ad}} n_i C_{p,i} \, dT + \Delta H_{rxn} \right]$$

$$\boxed{T_{ad} = 2052.43 \text{ K}}$$

next, using CEA we get

$$\boxed{T_{ad} = 2040.47 \text{ K}}$$

(CEA results are in the appendix)

the error is

$$\boxed{error = 11.96 \text{ K}}$$

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the mole fractions for my & CEAs analyses

my	CEA
N_2: 0.74026	N_2: 0.72918
O_2: 0.03935	O_2: 0.03746
CO_2: 0.09445	CO_2: 0.09354
H_2O: 0.12593	H_2O: 0.12422

For all product elements they are close to identical with approximately 1% difference.

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Problem 3. Adiabatic flame temperature and chemical equilibrium

A combustor uses gaseous hydrogen and gaseous oxygen as propellants. They are injected at 300K and a mixture ratio O/F = 12.0. The chamber pressure is 100 atm. Spectroscopy is used to measure the number density of a few specific species in the chamber. From these limited number of measurements, the conditions of equilibrium can be used to calculate the temperature of the products and the partial pressures and mole fractions of the rest of the species. Refer to the table provided in the notes (Lecture 7-8, page 10) for equilibrium constants, K_p, as function of temperature for the HO system of reactions.

    a. Write a balanced equation for the primary reaction (reaction a on the table) at O/F = 12.0. In this case, the products will comprise H_2O and what is left over from the excess reactants. Calculate the equivalence ratio.

    b. Calculate the adiabatic flame temperature based on the reaction in part a. Use either of the approaches from Problem 2.

    c. The measured number densities were used to yield these estimates of mole fraction
      H: 0.0124   OH: 0.1186 O_2: 0.1683   O: 0.0232
      Use their mole fractions to calculate the partial pressure of each of these species. Use the partial pressures along with the tabulated values for $K_p(T)$ to estimate the temperature of the gas in the chamber. Note that the measurements are not perfect and there will be some error in their values, and all the calculated K_p's will not necessarily yield the exact same temperature. Calculate the partial pressure of H_2O.

    d. What are the sources of the difference between temperatures calculated in b and c?

(a) O_2 & H_2 OH system equations

$$\boxed{H_2(g) + 0.5\,O_2(g) = H_2O(g)}$$

stoichiometric

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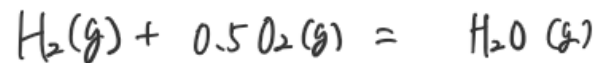
if $(O/F)_{op} = 12.0$

since $(O/F)_{stoich} = \dfrac{(0.5\,mol)(32\,g/mol)}{(1\,mol)(2\,g/mol)} = 8$

then $\quad \varphi = \dfrac{(O/F)_{stoich}}{(O/F)_{op}} = \dfrac{8}{12.0} = \boxed{0.6667}$

thus, there is $\dfrac{1}{0.6667} = 1.5$ times more O_2 than H_2

the balanced equation becomes

$$\boxed{H_2(g) + 0.75\,O_2(g) = H_2O(g) + 0.25\,O_2(g)}$$

(b) First calculate ΔH°_{rxn}

ΔH for $H = 218.00\,kJ/mol$, $OH = 38.99\,kJ/mol$, $O = 249.18\,kJ/mol$

from NIST dataset

$\Delta H_{rxn} = (1\,mol)(-241.826\,kJ/mol) = \boxed{-241.826\,kJ/mol}$

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then using the same approach in problem 2 (matlab)

where $T_{ref} = 300 K$

$\bar{C}_{p_i}$: functions from textbook

$$\Downarrow$$

$$abs\left[\sum_{products, i} \int_{T_{ref}}^{T_{ad}} n_i C_{p,i} \, dT + \Delta H_{rxn}\right]$$ minimize this

MATLAB gives the answer

$\quad T_{ad} = 4358.82 K$

However, CEA gives

$\quad T_{ad} = 3559.29 K$

The products OH, O, H, H_2O_2, H_2 distinguish the two results.

(c) The partial fractions are

$$P_H = (0.0124)(100 \text{ atm}) = 1.24 \text{ atm}$$

$$P_{OH} = (0.1186)(100 \text{ atm}) = 11.86 \text{ atm}$$

$$P_{O_2} = (0.1683)(100 \text{ atm}) = 16.83 \text{ atm}$$

$$P_O = (0.0232)(100 \text{ atm}) = 2.32 \text{ atm}$$

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now let's calculate K_p with our pressure values

say $p^0 :=$ reference pressure $= 1$ atm

$$H_2(g) + 0.75 O_2(g) = H_2O(g) + 0.25 O_2(g)$$
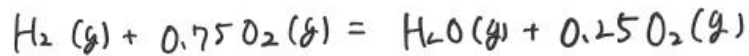
from this rxn we have the system of 0H rxns

$$
\begin{cases}
H_2 + 0.5 O_2 = H_2O & \cdots \; ⓪ \\
0.5 O_2 + 0.5 H_2 = OH & \cdots \; ① \\
0.5 H_2 = H & \cdots \; ② \\
0.5 O_2 = O & \cdots \; ③
\end{cases}
$$
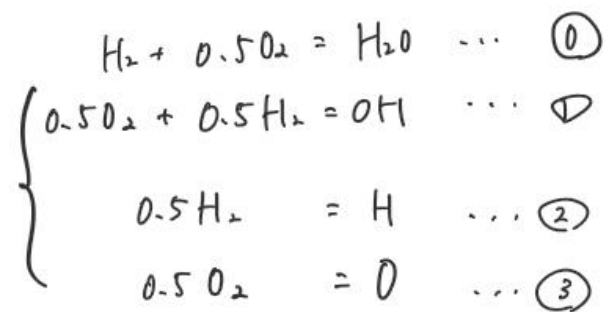
$$K_{p_0} = \frac{\left(P_{H_2O}/p^0 \right)}{\left(P_{H_2}/p^0 \right)\left(P_{O_2}/p^0 \right)^{1/2}} \qquad \cdots \; Ⓐ$$

same

$$K_{p_1} = \frac{P_{OH}/p^0}{\left(P_{H_2}/p^0 \right)^{0.5}\left(P_{O_2}/p^0 \right)^{0.5}} \qquad \cdots \; Ⓑ$$

$$K_{p_2} = \frac{P_H/p^0}{\left(P_{H_2}/p^0 \right)^{0.5}} \qquad \cdots \; Ⓒ$$

$$K_{p_3} = \frac{P_O/p^0}{\left(P_{O_2}/p^0 \right)^{0.5}} \qquad \cdots \; Ⓓ$$

$\sim$ $=$ known

$\sim$ $=$ unknown

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from ⓓ

$$K_{p3} = \frac{\left(2.32\ atm\Big/atm\right)}{\left(16.83\ atm\Big/atm\right)^{0.5}}$$

$$\approx 0.56552$$

using table on slides interpolate to get
Temperature value   (Matlab : with code)

Effect of Temperature on Equilibrium
HO System of Equations, $H_2 + \frac{1}{2} O_2 = H_2O$

| T (K)	$K_{p,a}$	$K_{p,b}$	$K_{p,c}$	$K_{p,d}$
298	1.1143×10^{40}	2.8340×10^{-7}	2.4831×10^{-36}	4.8978×10^{-41}
300	6.1235×10^{39}	3.1311×10^{-7}	4.2560×10^{-36}	9.0157×10^{-41}
400	1.7418×10^{29}	2.1419×10^{-5}	1.3459×10^{-26}	5.5335×10^{-30}
500	7.6913×10^{22}	2.6984×10^{-4}	6.9984×10^{-21}	7.7140×10^{-23}
1000	1.1482×10^{10}	4.1295×10^{-2}	2.2693×10^{-9}	1.9055×10^{-10}
1500	5.2541×10^{5}	2.1324×10^{-1}	1.7575×10^{-5}	1.6315×10^{-5}
2000	3.3931×10^{3}	4.7664×10^{-1}	1.6233×10^{-3}	7.3350×10^{-4}
2500	1.6127×10^{2}	7.6648×10^{-1}	2.5090×10^{-2}	1.5574×10^{-2}
3000	2.0999×10^{1}	1.0478	1.5762×10^{-1}	1.2010×10^{-1}
3500	4.9295	1.3046	5.8993×10^{-1}	5.1807×10^{-1}
4000	1.6623	1.5315	1.5933	1.5528
4500	7.0307×10^{-1}	1.7322	3.4602	3.6521
5000	3.5465×10^{-1}	1.9067	6.4506	7.2395

↑	↑	↑	↑
$H_2 + \frac{1}{2} O_2 = H_2O$	$\frac{1}{2} O_2 + \frac{1}{2} H_2 = OH$	$\frac{1}{2} H_2 = H$	$\frac{1}{2} O_2 = O$
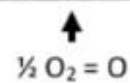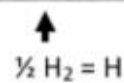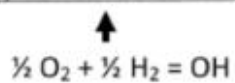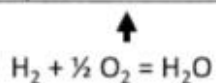
→ interpolating with these values

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$$\boxed{T = 3522.9 \text{ K}}$$

from this interpolate again to find

K_{p0}, K_{p1} & K_{p2} (using MATLAB)

this becomes

$$K_{p2} = 0.6359$$
$$K_{p1} = 1.3150$$
$$K_{p0} = 4.7799$$

Calculate P_{H_2} using these values

$$(P_{H_2})_2 = p^0 \left[\frac{\left(P_H / p^0 \right)}{K_{p2}} \right]^2$$

$$= (1 \, atm) \left[\frac{\left(\frac{1.24 \, atm}{1 \, atm} \right)}{0.6359} \right]^2$$

$$\approx 3.8025 \, atm$$

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$$(P_{H_2})_1 = P^0 \left[\frac{P_{OH}/P^0}{K_{P1} \left(P_{O_2}/P^0 \right)^{0.5}} \right]^2$$

$$= (1 \text{ atm}) \left[\frac{11.86\text{atm}/1\text{atm}}{(1.3150)\left(16.83\text{atm}/1\text{atm}\right)^{0.5}} \right]^2$$

$$\simeq 4.8332 \text{ atm}$$

take the average

$$P_{H_2} = \frac{(P_{H_2})_1 + (P_{H_2})_2}{2} = 4.31785 \text{ atm}$$

thus,

$$P_{H_2O} = K_{P_0} \cdot P^0 \left(P_{H_2}/P^0 \right) \left(P_{O_2}/P^0 \right)^{0.5}$$

$$P_{H_2O} = K_{P_0} \, P_{H_2} \left(P_{O_2}/P^0 \right)^{0.5}$$

$$P_{H_2O} = (4.7799)(4.31785\text{atm}) \left(\frac{16.83 \text{ atm}}{1 \text{ atm}} \right)^{0.5}$$

$$\boxed{P_{H_2O} = 84.67 \text{ atm}}$$

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(d)

The sources of difference are the uncommon product elements such as O, H, OH, H_2O_2, etc. that alter the ΔH°_{rxn} and C_p integrations in the calculations.

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Appendix

>>Matlab Code

AAE339 matlab code

```matlab
clear all; close all; clc;
```

problem 2

```matlab
% Optimazation for the sum of integrals to equal the heat of reaction

[x,fval,exitflag,output,lambda,grad,hessian] = HW4_opt_T_ad_p2([301], [300],
[3500]);

vpa(x, 10)
```

problem 3

<b>

```matlab
% Optimazation for the sum of integrals to equal the heat of reaction

[x2,fval2,exitflag2,output2,lambda2,grad2,hessian2] = HW4_opt_T_ad_p3([301],
[300], [5000]);

vpa(x2, 10)
```

<c>

```matlab
% interpolating

T_chamber = two_point_interpolate(0.56552,0.51807,1.5528,3500,4000);

Kp2 = two_point_interpolate(3522.9,3500,4000,0.58993,1.5933);

Kp1 = two_point_interpolate(3522.9,3500,4000,1.3046,1.5315);

Kp0 = two_point_interpolate(3522.9,3500,4000,4.9295,1.6623);
```

```matlab
function obj = HW4_p2_objective(T_ad)
    % Functions for the Cp for each element in the product
    nitrogen_Cp = @(theta) 39.060-512.79*theta.^(-1.5)+1072.7*theta.^(-2)-
820.40*theta.^(-3);
    oxygen_Cp = @(theta) 37.432+0.020102*theta.^(1.5)-178.57*theta.^(-
1.5)+236.88*theta.^(-2);
    carbon_dioxide_Cp = @(theta) -3.7357+30.529*theta.^(0.5)-
4.1034*theta+0.024198*theta.^2;
```

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```matlab
    water_vapor_Cp = @(theta) 143.05-183.54*theta.^(0.25)+82.751*theta.^(0.5)-
3.6989*theta;

    % Moles
    n_n2 = 23.513;   %[moles]
    n_o2 = 1.25;
    n_co2 = 3;
    n_h2o = 4;

    T_ref = 278; %[K]
    theta_ref = T_ref/100;
    theta_ad = T_ad/100;
    % Summations of integrations
    H_rxn = (n_n2*integral(nitrogen_Cp,theta_ref,theta_ad) +
n_o2*integral(oxygen_Cp,theta_ref,theta_ad) + ...
                n_co2*integral(carbon_dioxide_Cp,theta_ref,theta_ad) +
n_h2o*integral(water_vapor_Cp,theta_ref,theta_ad))*100;
    obj = abs(H_rxn - 2.0447*10^6);
end




function [x,fval,exitflag,output,lambda,grad,hessian] = HW4_opt_T_ad_p2(x0,lb,ub)
%% Start with the default options
options = optimoptions('fmincon');
%% Modify options setting
options = optimoptions(options,'Display', 'off');
options = optimoptions(options,'PlotFcn', {  @optimplotfunccount
@optimplotfval });
options = optimoptions(options,'HessianApproximation', 'bfgs');
[x,fval,exitflag,output,lambda,grad,hessian] = ...
fmincon(@HW4_p2_objective,x0,[],[],[],[],lb,ub,[],options);




function obj = HW4_p3_objective(T_ad)
    % Functions for the Cp for each element in the product
    oxygen_Cp = @(theta) 37.432+0.020102*theta.^(1.5)-178.57*theta.^(-
1.5)+236.88*theta.^(-2);
    water_vapor_Cp = @(theta) 143.05-183.54*theta.^(0.25)+82.751*theta.^(0.5)-
3.6989*theta;
    %hydro_monoxide_Cp = @(theta) 81.546-
59.350*theta.^(0.25)+17.329*theta.^(0.75)-4.266*theta;
    %hydro_molecule_Cp = @(theta) 20.78603+4.850638*10.^(-10)*(theta/10)...
    %    -1.582916*10.^(-10)*(theta/10).^2+1.525102*10.^(-
11)*(theta/10).^3+3.196347*10.^(-11)*(theta/10).^2;

    % Moles
    n_o2 = 0.25;
```

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```matlab
    n_h2o = 1;

    T_ref = 300; %[K]
    theta_ref = T_ref/100;
    theta_ad = T_ad/100;
    % Summations of integrations
    H_rxn = (n_o2*integral(oxygen_Cp,theta_ref,theta_ad) +
n_h2o*integral(water_vapor_Cp,theta_ref,theta_ad))*100;
    obj = abs(H_rxn - 241.826*10^3);
end
```

```matlab
function [x,fval,exitflag,output,lambda,grad,hessian] = HW4_opt_T_ad_p3(x0,lb,ub)
%% Start with the default options
options = optimoptions('fmincon');
%% Modify options setting
options = optimoptions(options,'Display', 'off');
options = optimoptions(options,'PlotFcn', {  @optimplotfunccount
@optimplotfval });
options = optimoptions(options,'HessianApproximation', 'bfgs');
[x,fval,exitflag,output,lambda,grad,hessian] = ...
fmincon(@HW4_p3_objective,x0,[],[],[],[],lb,ub,[],options);
```

```matlab
function y = two_point_interpolate(x,x_low,x_high,y_low,y_high)
    slope = (y_high - y_low) / (x_high - x_low);
    y = slope * (x - x_low) + y_low;
end
```

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>>CEA results

For problem 2

```
****************************************************************************
**

        NASA-GLENN CHEMICAL EQUILIBRIUM PROGRAM CEA2, FEBRUARY 5, 2004
                  BY  BONNIE MCBRIDE AND SANFORD GORDON
      REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996


****************************************************************************
**




 ### CEA analysis performed on Sun 09-Feb-2020 17:49:04

 # Problem Type: "Rocket" (Infinite Area Combustor)

 prob case=1111_____7282 ro equilibrium

 # Pressure (1 value):
 p,atm= 1

 # Equivalence based on Fuel/Oxid. wt ratio (Eq 9.19*) (1 value):
 phi= 0.8

 # You selected the following fuels and oxidizers:
 reac
 fuel C3H8              mole=100.0000  t,k= 298.000
 oxid Air               mole=100.0000  t,k= 298.000

 # You selected these options for output:
 # short version of output
 output short
 # Proportions of any products will be expressed as Mole Fractions.
 # Heat will be expressed as siunits
 output siunits

 # Input prepared by this script:prepareInputFile.cgi

 ### IMPORTANT:  The following line is the end of your CEA input file!
 end




            THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM

          COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

 Pin =    14.7 PSIA
```

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```
CASE = 1111_____

              REACTANT                    MOLES      ENERGY        TEMP
                                                     KJ/KG-MOL      K
FUEL         C3H8                    100.0000000  -104691.036    298.000
OXIDANT      Air                     100.0000000     -129.895    298.000

O/F=   19.59862  %FUEL=  4.854693  R,EQ.RATIO= 0.800304  PHI,EQ.RATIO=
0.800000

                   CHAMBER   THROAT
Pinf/P              1.0000   1.8045
P, BAR             1.0132   0.56152
T, K               2040.47  1819.87
RHO, KG/CU M       1.7019-1 1.0584-1
H, KJ/KG           -119.53  -451.65
U, KJ/KG           -714.87  -982.18
G, KJ/KG          -19273.5 -17534.9
S, KJ/(KG)(K)       9.3871   9.3871

M, (1/n)            28.497   28.521
(dLV/dLP)t        -1.00047 -1.00011
(dLV/dLT)p          1.0156   1.0043
Cp, KJ/(KG)(K)      1.5938   1.4598
GAMMAs              1.2321   1.2521
SON VEL,M/SEC       856.4    815.0
MACH NUMBER         0.000    1.000

PERFORMANCE PARAMETERS

Ae/At                        1.0000
CSTAR, M/SEC                 1174.6
CF                           0.6939
Ivac, M/SEC                  1466.0
Isp, M/SEC                    815.0

MOLE FRACTIONS

*Ar               0.00877  0.00877
*CO               0.00088  0.00016
*CO2              0.09354  0.09434
*H                0.00003  0.00000
*H2               0.00025  0.00006
H2O               0.12422  0.12517
*NO               0.00347  0.00183
*N2               0.72918  0.73064
*O                0.00017  0.00004
*OH               0.00203  0.00075
*O2               0.03746  0.03824

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K
```

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For problem 3

```
*****************************************************************************
**

          NASA-GLENN CHEMICAL EQUILIBRIUM PROGRAM CEA2, FEBRUARY 5, 2004
                    BY  BONNIE MCBRIDE AND SANFORD GORDON
        REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996



*****************************************************************************
**




 ### CEA analysis performed on Tue 11-Feb-2020 13:09:56

 # Problem Type: "Rocket" (Infinite Area Combustor)

 prob case=1111_____1362 ro equilibrium

 # Pressure (1 value):
 p,atm= 100

 # Oxidizer/Fuel Wt. ratio (1 value):
 o/f= 12

 # You selected the following fuels and oxidizers:
 reac
 fuel H2                mole=100.0000  t,k= 300.000
 oxid O2                mole=100.0000  t,k= 300.000

 # You selected these options for output:
 # short version of output
 output short
 # Proportions of any products will be expressed as Mole Fractions.
 # Heat will be expressed as siunits
 output siunits

 # Input prepared by this script:prepareInputFile.cgi

 ### IMPORTANT:  The following line is the end of your CEA input file!
 end




            THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM

          COMPOSITION DURING EXPANSION FROM INFINITE AREA COMBUSTOR

 Pin =  1469.6 PSIA
 CASE = 1111_____
```

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```
              REACTANT                           MOLES        ENERGY       TEMP
                                                            KJ/KG-MOL        K
 FUEL         H2                              100.0000000      53.359    300.000
 OXIDANT      O2                              100.0000000      54.358    300.000


 O/F=   12.00000   %FUEL=  7.692308  R,EQ.RATIO= 0.661390  PHI,EQ.RATIO=
 0.661390


                    CHAMBER   THROAT
 Pinf/P             1.0000    1.7311
 P, BAR             101.33    58.531
 T, K               3559.29   3372.16
 RHO, KG/CU M       6.6625 0  4.1082 0
 H, KJ/KG           3.6042    -804.29
 U, KJ/KG           -1517.22  -2229.03
 G, KJ/KG           -46860.1  -45204.2
 S, KJ/(KG)(K)      13.1666   13.1666


 M, (1/n)           19.459    19.679
 (dLV/dLP)t         -1.02763  -1.02307
 (dLV/dLT)p         1.4934    1.4373
 Cp, KJ/(KG)(K)     6.4682    6.1769
 GAMMAs             1.1360    1.1341
 SON VEL,M/SEC      1314.4    1271.1
 MACH NUMBER        0.000     1.000


 PERFORMANCE PARAMETERS


 Ae/At                        1.0000
 CSTAR, M/SEC                 1940.3
 CF                           0.6551
 Ivac, M/SEC                  2392.0
 Isp, M/SEC                   1271.1



 MOLE FRACTIONS


 *H                0.01237   0.00967
 HO2               0.00070   0.00049
 *H2               0.03406   0.02853
 H2O               0.64249   0.66548
 H2O2              0.00009   0.00006
 *O                0.02327   0.01917
 *OH               0.11870   0.10357
 *O2               0.16832   0.17304

  * THERMODYNAMIC PROPERTIES FITTED TO 20000.K
```

Tomoki Koike   AAE339