SOLUTIONS MANUAL

to accompany

AN INTRODUCTION TO COMBUSTION: Concepts and Applications

Third Edition

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PREFACE

This solutions manual has been developed to supplement the third edition of *AN INTRODUCTION TO COMBUSTION: Concepts and Applications* by S. R. Turns. The solution to each problem is presented in the same format to encourage students to develop an organized approach to problem solving. Although a more detailed format could be adopted, the approach used here is, first, to present a list of given or readily obtained information; second, to list what is to be determined; third, to list the major assumptions; fourth to present the solution, being careful to indicate equation numbers and other references; and, lastly, to comment on the solution. This last step, frequently neglected by students, is quite important in that it can result in students reflecting on what they have learned from the problem, questioning their assumptions, and, in general, providing a wider context for the problem. The solution to each problem starts on a new page to facilitate copying and posting.

Solutions to the following problems have been corrected from previous editions: 4.7, 13.3, 13.4, 13.5, 13.9, and 15.4.

PROBLEM 2-1

GIVEN: Air with a molar composition of 79% N_2 and 21% O_2

FIND: The mass fraction of O_2 and N_2 in the air

APPROACH: This a simple conversion problem using:

$$MW_{mix} = \Sigma X_i MW_i \qquad \text{and} \qquad Y_i = X_i \frac{MW_i}{MW_{mix}}$$

Given the molar composition: $X_{N_2} = 0.79$ and $X_{O_2} = 0.29$

mixture molecular weight:

$$MW_{mix} = \Sigma X_i MW_i = X_{N_2} MW_{N_2} + X_{O_2} MW_{O_2}$$

$$= 0.79(28.013) + (0.21)(32) = 28.85 \; {}^{kg}/_{kmol}$$

mass fraction of O_2 and N_2

$$Y_{O_2} = X_{O_2}\left(\frac{MW_{O_2}}{MW_{mix}}\right) = 0.21\left(\frac{32}{28.85}\right) = 0.233$$

$$Y_{N_2} = X_{N_2}\left(\frac{MW_{N_2}}{MW_{mix}}\right) = 0.79\left(\frac{28.013}{28.85}\right) = 0.767$$

Comments: Note that $Y_{O_2} > X_{O_2}$ since $MW_{O_2} > MW_{mix}$ and that $\Sigma Y_i = 1$ as would be expected.

PROBLEM 2-2

GIVEN: The following mixture:

Species	# MOLES	X_i	Y_i	MW_i
CO	0.095	0.002	0.002	28.010
CO_2	6	0.127	0.195	44.011
H_2O	7	0.149	0.094	18.016
N_2	34	0.722	0.707	28.013
NO	0.005	106×10^{-6}	111×10^{-6}	30.006
TOTAL:	47.1	1.0	1.0	

FIND: a) The mole fraction, mole %, and ppm of NO in the mixture
b) Determine the MW of the mixture
c) Determine the mass fraction of each constituent

a) $X_i = \dfrac{N_i}{\Sigma N_i} = \dfrac{N_{NO}}{N_{CO} + N_{CO_2} + N_{H_2O} + N_{N_2} + N_{NO}} = \dfrac{0.005}{0.095 + 6 + 7 + 34 + 0.005}$

$$\boxed{X_{NO} = 106 \times 10^{-6} \; Kmol/Kmol\text{-}mix}$$

$$\boxed{MOLE \% = X_i \cdot 100 = 0.0106 \%}$$

$PPM = \dfrac{\# NO}{TOT \#}(1 \times 10^6) = \dfrac{N_{NO} \cdot A}{\Sigma N_i \cdot A}(1 \times 10^6) = X_{NO}(1 \times 10^6) = \boxed{106 \; ppm}$

where $A \equiv$ Avogadro's Number

b) $MW_{mix} = \Sigma X_i MW_i = X_{CO} MW_{CO} + X_{CO_2} MW_{CO_2} + X_{H_2O} MW_{H_2O} + X_{N_2} MW_{N_2} + X_{NO} MW_{NO}$

where $X_{CO}, X_{CO_2}, X_{H_2O},$ and X_{N_2} are found in the same manner as X_{NO} was found

$MW_{mix} = (0.002)(28.010) + (0.127)(44.011) + (0.149)(18.016) + 0.722(28.013) + (106 \times 10^{-6})(33.006)$

$$\boxed{MW_{mix} = 28.6 \; Kg/Kmol\text{-}mix}$$

c) $Y_i = X_i \dfrac{MW_i}{MW_{mix}}$ $\longrightarrow$

$\left(Kg_i/Kg_{mix}\right)$

CO: $Y = (0.002)(28.01/28.6) = 0.002$

CO_2: $Y = (0.127)(44.011/28.6) = 0.195$

H_2O: $Y = (0.149)(18.016/28.6) = 0.094$

N_2: $Y = (0.722)(28.013/28.6) = 0.707$

NO: $Y = (106 \times 10^{-6})(30.006/28.6) = 111 \times 10^{-6}$

COMMENTS: Note that $ppm = X_i (1 \times 10^6)$ and that $\Sigma X_i = 1$ and $\Sigma Y_i = 1$ can often be used to check your calculations

PROBLEM 2-3

GIVEN : mixture with 5 kmole H_2 and 3 kmole O_2

FIND : χ_{H_2}, χ_{O_2}, MW_{mix}, Y_{H_2}, Y_{O_2}

SOLUTION :

a) $\chi_i = \dfrac{N_i}{N_{tot}}$; $\chi_{H_2} = \dfrac{5}{5+3} = \boxed{0.625}$

$\chi_{O_2} = 1 - \chi_{H_2} = 1 - 0.625 = \boxed{0.375}$

b) $MW_{mix} = \sum \chi_i MW_i = \chi_{H_2} MW_{H_2} + \chi_{O_2} MW_{O_2}$

$= 0.625 (2.016) + .375 (31.999)$

$\boxed{MW_{mix} = 13.260}$

c) $Y_i = \chi_i \dfrac{MW_i}{MW_{mix}}$; $Y_{H_2} = 0.625 \dfrac{2.016}{13.260} = \boxed{0.095}$

$Y_{O_2} = 1 - Y_{H_2} = 1 - 0.095 = \boxed{0.905}$

COMMENT : Even though the mole fraction of H_2 is large, its low molecular weight results in its having a small mass fraction.

GIVEN: $O_2 - CH_4$ mixture @ 300 K & 100 kPa;

$\chi_{O_2} = 0.2$

FIND: Y_{CH_4}, $N_{CH_4}/\forall$

ASSUMPTIONS: ideal gas mixture

SOLUTION:

a) $Y_{CH_4} = \chi_{CH_4} \dfrac{MW_{CH_4}}{MW_{mix}}$

$= \chi_{CH_4} \dfrac{MW_{CH_4}}{\chi_{CH_4} MW_{CH_4} + (1 - \chi_{CH_4}) MW_{O_2}}$

$= 0.2 \dfrac{16.043}{0.2(16.043) + 0.8(31.999)} = \dfrac{0.2(16.043)}{28.808}$

$\boxed{Y_{CH_4} = 0.111}$

b) $P_{CH_4} \forall = N_{CH_4} R_u T$; $P_{CH_4} = \chi_{CH_4} P$

$N_{CH_4}/\forall = \dfrac{\chi_{CH_4} P}{R_u T}$

$= \dfrac{(0.2) 100 \cdot 10^3}{8315 (300)} = \boxed{8.018 \cdot 10^{-3} \dfrac{kmol}{m^3}}$

COMMENT: Careful treatment of units is required in part b.

PROBLEM 2-5

GIVEN: $N_2 - Ar$ mixture with $N_{N_2} = 3 N_{Ar}$;
$T = 500 K$; $P = 250 kPa$

FIND: χ_i, MW_{mix}, Y_i, $N_{N_2}/\forall$

ASSUMPTION: ideal gas mixture

SOLUTION:

a) $\chi_{N_2} = \dfrac{N_{N_2}}{N_{MIX}} = \dfrac{3 N_{Ar}}{3 N_{Ar} + N_{Ar}} = \dfrac{3}{4} = \boxed{0.75}$

$\chi_{Ar} = 1 - 0.75 = \boxed{0.25}$

b) $MW_{mix} = \sum \chi_i MW_i$

$= 0.75 (28.014) + 0.25 (39.948)$

$\boxed{MW_{mix} = 30.998}$

c) $Y_{N_2} = \chi_{N_2} \dfrac{MW_{N_2}}{MW_{mix}} = 0.75 \dfrac{28.014}{30.998} = \boxed{0.678}$

$\boxed{Y_{Ar} = 1 - Y_{N_2} = 0.322}$

d) $P_{N_2} \forall = N_{N_2} R_u T$; $P_{N_2} = \chi_{N_2} P_{tot}$

$N_{N_2}/\forall = \dfrac{\chi_{N_2} P_{tot}}{R_u T} = \dfrac{(0.75) 250 \cdot 10^3}{8315 (500)} = \boxed{\begin{array}{c} 0.0451 \\ kmol_{N_2}/m^3 \end{array}}$

COMMENT: Careful treatment of units is required in part d.

GIVEN: $CO_2 - O_2$ mixture with $\chi_{CO_2} = 0.1$; $\chi_{O_2} = 0.9$;
$T = 400 K$

FIND: Standardized enthalpy of mixture

ASSUMPTION: Ideal-gas behavior

SOLUTION: This is a straightforward application of Eqn. 2.15a combined with the definition of standardized enthalpy (Eqn. 2.34).

$$\bar{h}_{CO_2} = \bar{h}^{\circ}_{f, CO_2} + \Delta \bar{h}_{s, CO_2} = -393,546 + 4003 \quad (\text{Table A.2})$$

$$= -389,543 \text{ kJ/kmol}$$

$$\bar{h}_{O_2} = \bar{h}^{\circ}_{f, O_2} + \Delta \bar{h}_{s, O_2} = 0 + 3031 = 3031 \text{ kJ/kmol}$$
$$(\text{Table A.11})$$

$$\bar{h}_{mix} = \sum \chi_i \bar{h}_i = \chi_{CO_2} \bar{h}_{CO_2} + \chi_{O_2} \bar{h}_{O_2} \quad (\text{Eqn. 2.15a})$$

$$= 0.1(-389,543) + 0.9(3031)$$

$$\boxed{\bar{h}_{mix} = -36,226 \text{ kJ/kmol}_{mix}}$$

COMMENT: The use of the Appendix A tables made this problem simple. Note that the same information is available as curvefit equations in Table A-13.

GIVEN: A stoichiometric mixture of methane and air

FIND: The mixture molecular weight

ASSUMPTIONS: Air consists of N_2 and O_2 and has the following composition: 21% O_2 and 79% N_2 by volume

APPROACH: Determine the stoichiometric ratio of air and fuel and then find the constituent mole fractions and MW_{mix}

Stoichiometric relation: $C_xH_y + a\,O_2 + 3.76a\,N_2 \longrightarrow x\,CO_2 + \frac{y}{2}\,H_2O + 3.76a\,N_2$

methane: $x=1$, $y=4$ $\longrightarrow$ $a = x + \frac{y}{4} = 2$

so the air-fuel stoichiometric mixture is

$$1\,CH_4 + 2\,O_2 + 7.52\,N_2$$

$N_{CH_4} = 1$ $\qquad X_{CH_4} = \dfrac{N_{CH_4}}{N_{TOT}} = \dfrac{N_{CH_4}}{N_{CH_4} + N_{O_2} + N_{N_2}} = \dfrac{1}{10.52} = 0.095$

$N_{O_2} = 2$ $\qquad X_{O_2} = \dfrac{N_{O_2}}{N_{TOT}} = \dfrac{2}{10.52} = 0.190$

$N_{N_2} = 7.52$ $\qquad X_{N_2} = \dfrac{N_{N_2}}{N_{TOT}} = \dfrac{7.52}{10.52} = 0.715$

$MW_{mix} = \sum X_i\,MW_i = X_{CH_4}\,MW_{CH_4} + X_{O_2}\,MW_{O_2} + X_{N_2}\,MW_{N_2}$

$\qquad = (0.095)(16.043) + (0.190)(32) + (0.715)(28.013)$

$$\boxed{MW_{mix} = 27.6 \; {}^{Kg}/_{Kmole}}$$

COMMENTS: If this was a fuel-rich or fuel-lean mixture,

$\qquad a = \dfrac{x + y/4}{\phi}$ $\qquad$ where $\phi \equiv$ equivalence ratio

PROBLEM 2-8

GIVEN: A stoichiometric air-propane (C_3H_8) mixture

FIND: The stoichiometric A/F ratio (mass)

ASSUMPTIONS: Air is comprised of 79% N_2 and 21% O_2 by volume

APPROACH: Determine the molar A/F ratio and convert to mass A/F ratio

Stoichiometric relation: $C_3H_8 + a O_2 + 3.76a N_2 \rightarrow 3CO_2 + 4H_2O + 3.76a N_2$

$$a = \frac{x + y/4}{\phi} \qquad x = 3, \ y = 8, \ \phi = 1$$

$$a = 5$$

Molar A/F ratio: $A/F = \dfrac{a + 3.76a}{1} = \dfrac{4.76a}{1}$

Mass A/F ratio = $\left(\dfrac{A}{F}\right)_{MOLAR} \left(\dfrac{MW_{air}}{MW_{fuel}}\right) = 4.76a \left(\dfrac{MW_{air}}{MW_{fuel}}\right)$

$$\left(\frac{A}{F}\right)_{MASS} = 4.76(5)\left(\frac{28.85}{44.096}\right)$$

$$\boxed{\left(\frac{A}{F}\right)_{MASS} = 15.6}$$

GIVEN: Propane (C_3H_8) burning at an air-fuel ratio (mass) of 18:1

FIND: The equivalence ratio, ϕ

ASSUMPTIONS: Air is comprised of 79% N_2 and 21% O_2 by volume

APPROACH: Determine the stoichiometric A/F ratio and then the equivalence ratio

Stoichiometric relation: $C_3H_8 + aO_2 + 3.76aN_2 \rightarrow 3CO_2 + 4H_2O + 3.76aN_2$

$$a = \frac{x + y/4}{\phi} \qquad x=3, \, y=8, \, \phi=1 \qquad a=5$$

$$\left. A/F \right)_{STOICH} = 4.76a \left(\frac{MW_{air}}{MW_{fuel}} \right) = 4.76 (5) \left(\frac{28.85}{44.096} \right) = 15.6$$

Equivalence ratio:

$$\phi = \frac{\left(A/F \right)_{STOICH}}{\left(A/F \right)_{ACTUAL}} = \frac{15.6}{18.0} = 0.87$$

$$\boxed{\phi = 0.87}$$

COMMENTS: Since $\phi < 1$ this combustion process is fuel-lean. Also note that ϕ does not depend on whether the A/F ratios are expressed in terms of moles or mass since ϕ is also a ratio

PROBLEM 2-10

GIVEN: An equivalence ratio of 0.6

FIND: The corresponding A/F ratios (mass) for methane (CH_4), propane (C_3H_8) and decane ($C_{10}H_{22}$)

ASSUMPTIONS: Air is comprised of 79% N_2 and 21% O_2 by volume

APPROACH: Use the relationships:

$$a = \frac{x + y/4}{\phi} \quad \text{and} \quad \left.\frac{A}{F}\right)_{Mass} = 4.76a \frac{MW_{air}}{MW_{fuel}}$$

methane (CH_4) $x=1$, $y=4$, $MW = 16.043 \frac{kg}{kmole}$

$$a = \frac{1 + 4/4}{0.6} = 3.33 \longrightarrow \left.\frac{A}{F}\right)_{mass} = 4.76(3.33)\left(\frac{28.85}{16.043}\right)$$

$$\boxed{\left.\frac{A}{F}\right)_{mass} = 28.50 \; {}^{kg\cdot air}/_{kg\cdot fuel}}$$

propane (C_3H_8) $x=3$, $y=8$, $MW = 44.096 \frac{kg}{kmole}$

$$a = \frac{3 + 8/4}{0.6} = 8.33 \longrightarrow \left.\frac{A}{F}\right)_{mass} = 4.76(8.33)\left(\frac{28.85}{44.096}\right)$$

$$\boxed{\left.\frac{A}{F}\right)_{mass} = 25.94 \; {}^{kg\cdot air}/_{kg\cdot fuel}}$$

decane ($C_{10}H_{22}$)

$$a = \frac{10 + 22/4}{0.6} = 25.83 \longrightarrow \left.\frac{A}{F}\right)_{mass} = 4.76(25.83)\left(\frac{28.85}{142.284}\right)$$

$$\boxed{\left.\frac{A}{F}\right)_{mass} = 24.93 \; {}^{kg\cdot air}/_{kg\cdot fuel}}$$

COMMENTS: Note how the A/F ratio (mass) changes only slightly from one hydrocarbon fuel to another. while the A/F ratio (molar) varies from 15.9 (methane) to 123 (decane). This difference in behavior is due to the MW_{fuel} increasing as the molar A/F ratio increases.

PROBLEM 2-11

GIVEN: 3% (by volume) O_2 measured in the exhaust of a propane (C_3H_8) - fueled truck

FIND: The air - fuel ratio (mass) supplied to the engine

ASSUMPTIONS: Complete combustion with no dissociation

APPROACH: Use conservation of O atoms to determine the A/F ratio from the exhaust oxygen mole fraction

assumed combustion reaction: $C_3H_8 + aO_2 + 3.76aN_2 \rightarrow 3CO_2 + 4H_2O + bO_2 + 3.76aN_2$

conservation of O atoms:
$$2a = 3(2) + 4 + b(2)$$
$$a = 5 + b$$
$$b = a - 5$$

exhaust O_2 mole fraction:

$$X_{O_2} = \frac{N_{O_2}}{N_{CO_2} + N_{H_2O} + N_{O_2} + N_{N_2}} = \frac{b}{3 + 4 + b + 3.76a}$$

using $b = a - 5$:

$$X_{O_2} = \frac{a-5}{4.76a + 2} \longrightarrow a = \frac{5 + 2X_{O_2}}{1 - 4.76X_{O_2}}$$

exhaust O_2 3% (by volume) $\longrightarrow$ $X_{O_2} = 0.03$

$$a = \frac{5 + 2(0.03)}{1 - 4.76(0.03)} = 5.90$$

$$\frac{A}{F}\Big)_{mass} = 4.76a\left(\frac{MW_{air}}{MW_{fuel}}\right) = 4.76(5.90)\left(\frac{28.85}{44.096}\right)$$

$$\boxed{\frac{A}{F}\Big)_{MASS} = 18.37}$$

COMMENTS: This engine is running at a fuel-lean condition
$$a = \frac{x + y/4}{\phi} \longrightarrow \phi = \frac{x + y/4}{a} = \frac{5}{5.9} = 0.85$$

PROBLEM 2-12

GIVEN: 1 mole of alcohol $(C_x H_y O_z)$ undergoing complete combustion

FIND: Stoichiometric balance equation and number of moles of air to burn 1 mole of alcohol

ASSUMPTIONS: no dissociation and air that is 79% N_2 and 21% O_2 (vol)

APPROACH: Use conservation of elements for the combustion of one mole of alcohol

Stoichiometric balance:

$$C_x H_y O_z + a O_2 + 3.76a\, N_2 \longrightarrow b\, CO_2 + c\, H_2O + 3.76a\, N_2$$
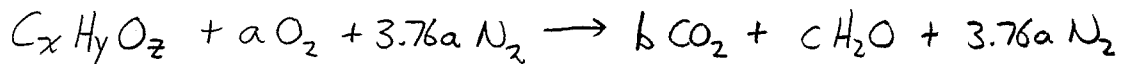
conservation of carbon: $\quad x = b \longrightarrow \boxed{b = x}$

conservation of H : $\quad y = 2c \longrightarrow \boxed{c = y/2}$

conservation of O : $\quad z + 2a = 2b + c = 2x + y/2$

$$\boxed{a = x + y/4 - z/2}$$

number of moles of air to burn 1 mole of alcohol:

$$\frac{N_{AIR}}{N_{fuel}} = \frac{a + 3.76a}{1} = 4.76a$$

$$\boxed{\frac{N_{AIR}}{N_{fuel}} = 4.76\left[x + y/4 - z/2\right]}$$

COMMENTS: Note that stoichiometric combustion of an alcohol $(C_x H_y O_z)$ requires less oxygen than the combustion of a comparable hydrocarbon fuel $(C_x H_y)$ due to the presence of oxygen in the fuel

PROBLEM 2-13

GIVEN: Methanol (CH_3OH) and the results of problem 2-8

FIND: The stoichiometric A/F ratio (mass) and compare with that of methane.

APPROACH: Use the relationship developed in problem 2-8 for both methanol and methane

methanol (CH_3OH) : $C_x H_y O_z$ $x=1, y=4, z=1$
MW = 32 kg/kmole

$$\left.\frac{A}{F}\right)_{MASS} = 4.76 \left[x + y/4 - z/2 \right] \left(\frac{MW_{air}}{MW_{fuel}} \right)$$

$$= 4.76 \left[1 + 4/4 - 1/2 \right] \left(\frac{28.85}{32} \right) = 6.4$$

$$\boxed{\left.\frac{A}{F}\right)_{MASS} = 6.4}$$

methane (CH_4) : $C_x H_y O_z$ $x=1, y=4, z=0$
MW = 16 kg/kmole

$$\left.\frac{A}{F}\right)_{MASS} = 4.76 \left[x + y/4 - z/2 \right] \left(\frac{MW_{air}}{MW_{fuel}} \right)$$

$$= 4.76 \left[1 + 4/4 - 0 \right] \left(\frac{28.85}{16} \right)$$

$$\boxed{\left.\frac{A}{F}\right)_{MASS} = 17.2}$$

COMMENTS: The large difference in the A/F ratios for methanol and methane is primarily due to the differences in fuel MW. On a molar basis the A/F ratio for methanol is 7.14 and 9.52 for methane.
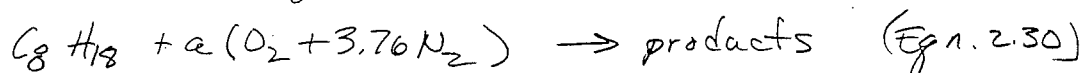
PROBLEM 2-14

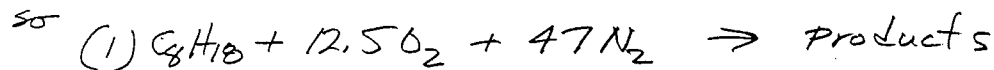GIVEN: Stoichiometric mixture of isooctane & air

FIND: H per kmol of $C_8 H_{18}$; $\bar{h}_{mix}$; h_{mix}.

ASSUMPTIONS: Air is 79% N_2 & 21% O_2; ideal gas

APPROACH: We start by finding the stoichiometric proportions of each component:

$$C_8 H_{18} + a(O_2 + 3.76 N_2) \longrightarrow \text{products} \quad (Eqn. 2.30)$$

$$a = x + y/4 = 8 + 18/4 = 12.5 \quad (Eqn. 2.31)$$

so

$$(1) C_8 H_{18} + 12.5 O_2 + 47 N_2 \Longrightarrow \text{Products}$$

As the above is written for 1 kmol of $C_8 H_{18}$,

a) $H = (1) \bar{h}_{C_8 H_{18}} + 12.5 \bar{h}_{O_2} + 47 \bar{h}_{N_2}$ [=] J/kmol-$C_8 H_{18}$

At 298 K, $\bar{h}_{\underset{octane}{iso-}} = -224,109$ kJ/kmol (Evaluated from curvefit coefficients in Table B.2)

$$\bar{h}_{O_2} = \bar{h}^{\circ}_{f,O_2} = 0$$

$$\bar{h}_{N_2} = \bar{h}_{f,O_2} = 0$$

$$\boxed{H \text{ (kJ/kmol-}C_8 H_{18})} = (1)(-224,109) + 12.5(0) + 47(0)$$

$$= \boxed{-224,109}$$

b) $\bar{h}_{mix} = \Sigma \chi_i \bar{h}_i$; $\chi_i = N_i / N_{tot}$

$$\chi_{C_8 H_{18}} = 1/(1 + 12.5 + 47) = 1/60.5 = 0.0165$$

$$\chi_{O_2} = 12.5(1 + 12.5 + 47) = 0.2066$$

$$\chi_{N_2} = 1 - \chi_{C_8 H_{18}} - \chi_{O_2} = 0.7769$$

$$\bar{h}_{mix} = 0.0165(-224,109) + 0.2066(0) + 0.7769(0)$$

$$\boxed{\bar{h}_{mix} = -3700 \quad kJ/kmol\text{-}mix}$$

c) $h_{mix} = \sum Y_i h_i = \bar{h}_{mix}/MW_{mix}$

$MW_{mix} = \sum x_i MW_i$

$$= 0.0165(114.230) + 0.2066(31.999) +$$
$$0.7769(28.014) = 30.260$$

$$\boxed{h_{mix}} = \frac{-3698}{30.260} = \boxed{-122.2 \quad kJ/kg\text{-}mix}$$

COMMENTS: We note that although both n-octane and isooctane are represented as C_8H_{18}, they have different molecular structures as discussed in the Chapter 2 Appendix. Because of these structural differences, the enthalpy-of-formations of the two compounds have different values. Table B.2 was used to calculate $\bar{h}_f^0$ for isooctane as the value given in Table B.1 is for n-octane. Spreadsheet software simplifies calculating properties from the Table B.2 curvefit coefficients.

PROBLEM 2-15

GIVEN: Isooctane-air, $\phi = 1$, $T = 500K$

FIND: H (per kmol C_8H_{18}), $\bar{h}_{mix}$, h_{mix}

ASSUMPTIONS: Air is 79% N_2 & 21% O_2; ideal gas.

APPROACH: We need only evaluate the enthalpies of the constituents at 500K and then follow the solution to Prob. 2-14.

	$\bar{h}_f$	$\Delta\bar{h}_s$ @ 500K	$\bar{h}(500K)$	
Isooctane	—	—	−175,807	Table B.2*
O_2	0	6097	6097	Table A.11
N_2	0	5920	5920	Table A.7

*Evaluated using spreadsheet software

a) H (kJ/kmol C_8H_{18}) = $(1)(-175,807) + 12.5(6097) + 47(5920)$

$$\boxed{H = +178,646 \text{ kJ}} \text{ (for 1 mole } C_8H_{18})$$

b) $\bar{h}_{mix} = \dfrac{H}{N_{mix}} = \dfrac{178,646}{1 + 12.5 + 47} = \boxed{2953 \text{ kJ/kmol-mix}}$

c) $h_{mix} = \bar{h}_{mix}/MW_{mix} = \dfrac{2953}{30.260} = \boxed{97.59 \text{ kJ/kg-mix}}$

COMMENT: Note the use of Table B.2 in combination with Tables A.7 & A.11.

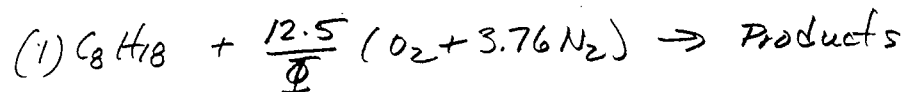GIVEN: Isooctane-air, $\bar{\Phi} = 0.7$, $T = 500K$

FIND: H (per kmol C_8H_{18}), $\bar{h}_{mix}$, h_{mix}

ASSUMPTIONS: see Prob. 2-14

APPROACH: After calculating the proportions of the constituents for $\Phi = 0.7$, we follow the same solution as for Prob. 2-17.

(1) $C_8H_{18} + \dfrac{12.5}{\Phi}(O_2 + 3.76 N_2) \Rightarrow$ Products

	N	χ	$\bar{h}(500K)$	
C_8H_{18}	1	0.0116	$-175,807$	
O_2	17.86	0.2077	6097	See Prob. 2-15
N_2	67.14	0.7807	5920	
$\sum N_i = 86.00$				

a) $H = 1(-175,807) + 17.86(6097) + 67.14(5920)$

$$\boxed{H = +330,554 \text{ kJ}} \quad \text{(for 1 kmol } C_8H_{18})$$

b) $\bar{h}_{mix} = \dfrac{H}{N_{MIX}} = \dfrac{330,554}{86} = \boxed{3844 \text{ kJ/kmol}-mix}$

c) $MW_{mix} = \sum \chi_i MW_i = 0.0116(114.230) + 0.2077(31.999)$
$$+ 0.7807(28.014) = 29.842$$

$h_{mix} = \dfrac{\bar{h}_{mix}}{MW_{mix}} = \dfrac{3844}{29.842} = \boxed{128.8 \text{ kJ/kg}-mix}$

COMMENT: Note how for non-stoichiometric combustion "a/Φ" is substituted for "a" in Eqn. 2.30. As expected, the mixture enthalpy increases with the addition of excess air.
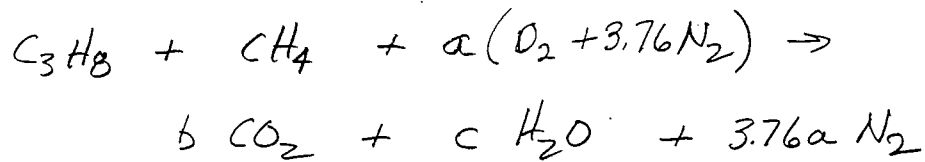
GIVEN: Equimolar mixture of C_3H_8 & CH_4 burning with air

FIND: N_F/N_A for $\phi = 1$ and $\phi = 0.8$

ASSUMPTIONS: Air is 79% N_2 & 21% O_2

APPROACH: C, H, & O element balances are req'd to determine the coefficient "a".

$$C_3H_8 + CH_4 + a(O_2 + 3.76N_2) \rightarrow$$
$$b\ CO_2 + c\ H_2O + 3.76a\ N_2$$

C: $3 + 1 = b$ $(b = 4)$
H: $8 + 4 = 2c$ $(c = 6)$
O: $2a = 2b + c = 2(4) + 6 = 14$
$$a = 7$$

a) For $\phi = 1$,

$$\frac{N_F}{N_A} = \frac{1+1}{7(4.76)} = \boxed{0.0600 \ \frac{kmol_{Fuel}}{kmol\ air}}$$

b) For $\phi = 0.8$

$$\frac{N_F}{N_A} = \phi\ (N_F/N_A)_{\phi=1} = 0.8(0.060) = \boxed{0.048 \ \frac{kmol_F}{kmol\ air}}$$

COMMENT: An alternative approach would be to define a composite fuel ($C_3H_8 + CH_4 \equiv C_4H_{12}$) and calculate "$a$" from Eqn. 2.31 ($a = x + y/4 = 4 + 12/4 = 7$).

GIVEN: Ideal (no dissociation) combustion products of C_8H_{18}-air for $\Phi = 0.7$, $T = 1000K$, $P = 1\,atm$
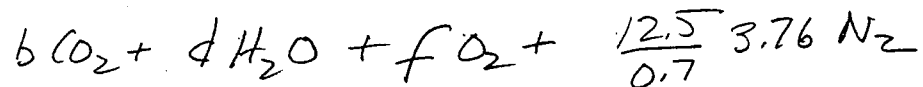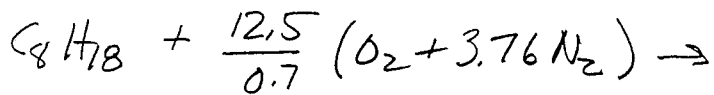
FIND: H_{prod} (per kmole C_8H_{18})

H_{prod} (per kg C_8H_{18})

h_{prod}

ASSUMPTIONS: No dissociation (given), ideal gas mixture

APPROACH: We first find the mixture composition & then calculate the mixture enthalpy.

Employing Eqn. 2.68, $a = (x + y/4)/\Phi$,

$$a = \frac{8 + 18/4}{0.7} = \frac{12.5}{0.7}. \quad Thus,$$

$$C_8H_{18} + \frac{12.5}{0.7}(O_2 + 3.76 N_2) \rightarrow$$

$$b\,CO_2 + d\,H_2O + f\,O_2 + \frac{12.5}{0.7}\,3.76\,N_2$$

C: $8 = b$ $(b = 8)$

H: $18 = 2d$ $(d = 9)$

O: $\left(\frac{12.5}{0.7}\right)2 = 2b + d + 2f$

$\qquad = 16 + 9 + 2f$

$$f = \frac{1}{2}\left(\frac{12.5}{0.7}2 - 16 - 9\right) = 5.357$$

$$N_{tot} = b + d + f + 3.76\,a$$

$$= 8 + 9 + 5.357 + 3.76\,\frac{12.5}{0.7}$$

$$= 89.50$$

Mole fractions, $x_i = N_i/N_{tot}$:

$$x_{CO_2} = 8/89.5 \quad = \quad = 0.0894$$

$$x_{H_2O} = 9/89.5 \quad\quad = 0.1006$$

$$x_{O_2} = 5.357/89.5 \quad = 0.0599$$

$$x_{N_2} = 67.14/89.5 \quad = \underline{0.7502}$$

$$\Sigma = 1.000$$

Species i	N_i	$\bar{h}_{f,i}^{\circ}$	$\Delta\bar{h}_{s,i}^{\circ}$ (1000K)	$N_i\,\bar{h}_i$ (1000K)
CO_2	8	-393,546	33,425	-2,880,968
H_2O	9	-241,845	25,993	-1,942,668
O_2	5.357	0	22,721	121,716
N_2	67.14	0	21,468	1,441,362

$$\Sigma N_i = 89.497$$

$$\Sigma N_i\,\bar{h}_i = -3,260,558$$

$$\boxed{H\left(\text{per } \frac{kmole}{C_8H_{18}}\right)} = \Sigma N_i\,\bar{h}_i = \boxed{-3,260,558 \ kJ}$$

$$\boxed{H\left(\text{per } \frac{kg}{C_8H_{18}}\right)} = \frac{\Sigma N_i\,\bar{h}_i}{MW_{C_8H_{18}}} = \frac{-3,260,558}{114.230} = \boxed{\begin{array}{c}-28,544 \\ kJ\end{array}}$$

PROBLEM 2-18 (Continued)

$$h_{prod} = \frac{\sum N_i \bar{h_i} / \sum N_i}{MW_{prod}}$$

$$MW_{prod} = \sum x_i MW_i$$
$$= 0.0894 (44.011) + 0.1006 (18.016)$$
$$\quad + 0.0599 (31.999) + 0.7502 (28.014)$$
$$= 28.68$$

$$\boxed{h_{prod}} = \frac{-3,260,558}{89.497 (28.68)} = \boxed{-1270 \quad kJ/kg\text{-}prod}$$
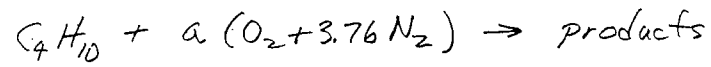
COMMENT: This problem illustrates calculation of product properties on a "fuel basis", i.e., per mole of fuel or mass of fuel.

GIVEN: C_4H_{10} - air, $\phi = 0.75$

FIND: N_A/N_F

SOLUTION:

$$C_4H_{10} + a(O_2 + 3.76\,N_2) \rightarrow \text{products}$$

For $\phi = 1$, $a = x + y/4 = 4 + 10/4 = 6.5$

$$\frac{N_A}{N_F} = \frac{4.76\,a}{\phi} = \frac{4.76\,(6.5)}{0.75} = \boxed{41.25}$$

GIVEN: $C_2H_4 - O_2$, $\Phi = 0.9$, $\dot{N}_{C_2H_4} = 30$ kmol/hr

FIND: a) $\dot{E}$ $(= \dot{m}_{C_2H_4} \ LHV)$

b) $\dot{N}_{O_2}$, $\dot{m}_{O_2}$

SOLUTION:

a) $\dot{E} = \dot{m}_{C_2H_4} \ LHV = \dot{N}_{C_2H_4} \ MW_{C_2H_4} \ LHV$

$= 30 \ \dfrac{kmol}{hr} \ \dfrac{1 \ hr}{3600 \ s} \ 28,054 \ \dfrac{kg}{kmol} \ 47,161 \ \dfrac{kJ}{kg}$

$\lfloor$ Table B.1

$= 11025 \ \dfrac{kJ}{s}$

$\boxed{\dot{E} = 11025 \ kW}$

$\dot{E} = 11025 \ kW \ \dfrac{1000 \ W}{kW} \ \dfrac{3.412 \ BTu/hr}{W}$

$\boxed{\dot{E} = 37.62 \cdot 10^6 \ \dfrac{BTu}{hr}} = 37.62 \ MM \ BTu/hr$

b) For stoichiometric conditions,

$C_2H_4 + a O_2 \rightarrow 2 CO_2 + 2 H_2 O$

O-balance: $2a = 4 + 2$; $a = 3$

$\dot{N}_{O_2} = \dot{N}_{C_2H_4} \ \dfrac{N_{O_2}}{N_{C_2H_4}} = \dot{N}_{C_2H_4} \ \dfrac{a}{\Phi}$

$\boxed{\dot{N}_{O_2}} = 30 \ \dfrac{kmol}{hr} \ \dfrac{3}{0.9} = \boxed{100 \ \dfrac{kmol}{hr}}$

$\boxed{\dot{m}_{O_2}} = \dot{N}_{O_2} \ MW_{O_2} = 100 \ \dfrac{kmol}{hr} \ \dfrac{1 \ hr}{3600 \ s} \ 31.999 \ \dfrac{kg}{kmol} = \boxed{0.889 \ \dfrac{kg}{s}}$

GIVEN: CH_3OH-air $(\Phi < 1)$; $A/F = 8 \, kg_F/kg_{air}$

FIND: Φ, χ_{CO_2}

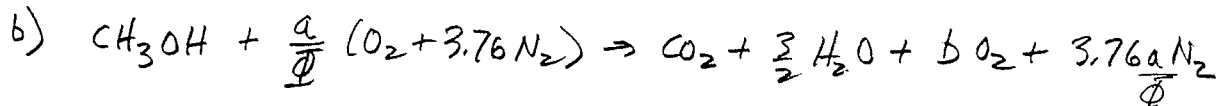ASSUMPTIONS: no dissociation; air is 79% N_2, 21% O_2.

SOLUTION: For $\Phi = 1$

a) $CH_3OH + a(O_2 + 3.76)N_2 \rightarrow CO_2 + \frac{3}{2}H_2O + 3.76a\,N_2$
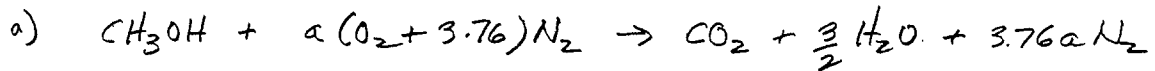
O-balance: $1 + 2a = 2 + 1.5$; $a = 2.5/2 = 1.25$

$$\left(A/F\right)_{\Phi=1} = \frac{4.76\,a\,MW_{air}}{MW_{CH_3OH}} \qquad (Eqn.\ 2.32)$$

$$= \frac{4.76\,(1.25)\,28.85}{32.040} = 5.358$$

$$\boxed{\Phi} = \frac{(A/F)_{\Phi=1}}{(A/F)} = \frac{5.358}{8} = \boxed{0.670} \qquad Eqn.\ 2.33a$$

b) $CH_3OH + \frac{a}{\Phi}(O_2 + 3.76\,N_2) \rightarrow CO_2 + \frac{3}{2}H_2O + b\,O_2 + \frac{3.76a}{\Phi}N_2$

O-balance: $1 + \frac{2a}{\Phi} = 2 + 1.5 + 2b$

$$b = \frac{1}{2}\left(\frac{2a}{\Phi} - 2.5\right) = \frac{a}{\Phi} - 1.25 = \frac{1.25}{0.67} - 1.25$$

$$b = 0.6157$$

$$\chi_{CO_2} = \frac{N_{CO_2}}{N_{tot}} = \frac{1}{1 + 1.5 + 0.6157 + 3.76(1.25)/0.67} = \frac{1}{10.131}$$

$$\boxed{\chi_{CO_2} = 0.0987}$$

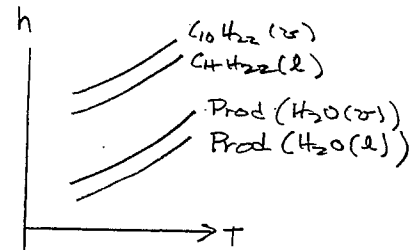COMMENT: O-element balances must account for oxygen content in the fuel.

PROBLEM 2-22

GIVEN: n-decane $LHV = 44,597$ kJ/kg (vapor)

n-decane $h_{fg} = 276.8$ kJ/kg

water $h_{fg} = 2442.2$ kJ/kg

FIND: a) LHV n-decane (liq.)
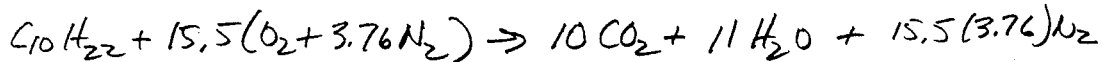
b) HHV n-decane (vap.)

SOLUTION:

a) LHV (liq.) $= LHV$ (vap.) $- h_{fg, C_{10}H_{22}}$

(see graph)

$\boxed{LHV(\ell)} = 44597 - 276.8 = \boxed{44,320 \text{ kJ/kg}}$

b) HHV (vap) $= LHV$ (vap) $+ \left(\dfrac{N_{H_2O}}{N_{C_{10}H_{22}}} \dfrac{MW_{H_2O}}{MW_{C_{10}H_{22}}} \right) h_{fg, H_2O}$

where the term in brackets is mass of H_2O per mass of $C_{10}H_{22}$. To find $N_{H_2O}/N_{C_{10}H_{22}}$, we write:

$C_{10}H_{22} + 15.5(O_2 + 3.76 N_2) \rightarrow 10 CO_2 + 11 H_2O + 15.5(3.76) N_2$

$\boxed{HHV(\text{vap})} = 44,597 + \dfrac{11}{1} \dfrac{18.016}{142.284} 2442.2 = \boxed{47,999 \text{ kJ/kg}}$

COMMENTS: Visualizing LHV, HHV graphically greatly aids in performing these computations. Note how the conversion from $LHV \Leftrightarrow HHV$ involves the mass ratio of water formed to fuel burned. The HHV-value of 47,999 kJ/kg is for practical purposes the same as the value given in Table B.1 ($HHV = 48,002$ kJ/kg).

GIVEN: The lower heating value for methane, $LHV = 50,016$ kJ/kg @ 298K

FIND: The enthalpy of formation of methane at 298 K

ASSUMPTIONS: complete combustion of methane to form CO_2, H_2O and N_2

APPROACH: Use the stoichiometric relation to determine the proper A/F ratio and combustion products for 1 Kmole of methane. Then use the first law of thermodynamics to evaluate the reactant enthalpy.

Stoichiometric relation

$$CH_4 + aO_2 + 3.76a\,N_2 \rightarrow CO_2 + 2H_2O + 3.76a\,N_2$$
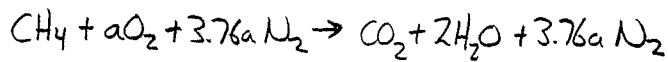
$$a = x + y/4 = 2$$
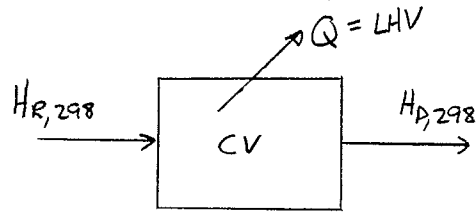
BASED ON FIRST LAW ANALYSIS OF CONTROL VOLUME (CV) at steady-state

$$H_{R,298} = H_{P,298} + LHV_{298}$$

$$H_{P,298} = 1\left[\bar{h}^{\circ}_{f_{298}} + \left(\bar{h} - \bar{h}^{\circ}_{f,298}\right)\right]_{CO_2} + 2\left[\bar{h}^{\circ}_f + \left(\bar{h} - \bar{h}^{\circ}_{f,298}\right)\right]_{H_2O} + 7.52\left[\bar{h}^{\circ}_{f_{298}} + \left(\bar{h} - \bar{h}^{\circ}_{f,298}\right)\right]_{N_2}$$

using appendix A - T = 298 K

$$H_{P,298} = 1\left[-393546 + 0\right] + 2\left[-241847 + 0\right] + 7.52\left[0 + 0\right] = -877240 \text{ KJ}$$

$$H_{R,298} = 1\left[\bar{h}^{\circ}_{f_{298}} + \left(\bar{h} - \bar{h}^{\circ}_{f,298}\right)\right]_{CH_4} + 2\left[\bar{h}^{\circ}_f + \left(\bar{h} - \bar{h}^{\circ}_{f,298}\right)\right]_{O_2} + 7.52\left[\bar{h}^{\circ}_{f,298} + \left(\bar{h} - \bar{h}^{\circ}_{f,298}\right)\right]_{N_2}$$

again using appendix A - T = 298 K

$$H_{R,298} = 1\left[\bar{h}^{\circ}_{f,298} + 0\right]_{CH_4} + 2\left[0 + 0\right]_{O_2} + 7.52\left[0 + 0\right]_{N_2} = 1\left[\bar{h}^{\circ}_{f,298}\right]_{CH_4}$$

$$H_R = 1\left[\bar{h}^{\circ}_{f,298}\right]_{CH_4} = H_{P,298} + LHV_{298} = -877240 \text{ KJ} + \left(50,016 \tfrac{KJ}{kg}\right)\left(\tfrac{16\,Kg}{Kmole}\right)\left(1\,Kmole\right)$$

$$\boxed{\left[\bar{h}^{\circ}_{f,298}\right]_{CH_4} = -76984 \text{ KJ/Kmole}}$$

GIVEN: The mixture composition in problem 2-2 at $T = 1000$ K

FIND: The absolute enthalpy of the mixture ($^{KJ}/_{kmol-mix}$)

APPROACH: Determine the absolute enthalpy of each species in the mixture using appendix A and then calculate the mixture absolute enthalpy from:

$$\bar{h}_{MIX} = \Sigma x_i \bar{h}_i$$

mixture composition (from problem 2-2) and species enthalpies (appendix A)

Species	#MOLES	x	$\bar{h}_{f,298}^{o}$ ($^{KJ}/_{kmol}$)	$(\bar{h}_{1000} - \bar{h}_{f,298}^{o})$ ($^{KJ}/_{kmole}$)
CO	0.095	0.002	-110541	21697
CO_2	6	0.127	-393546	33425
H_2O	7	0.149	-241847	25993
N_2	34	0.722	0	21468
NO	0.005	106×10^{-6}	90297	22241

$$\bar{h}_{mix} = \Sigma x_i \bar{h}_i \quad \text{where} \quad \bar{h}_i = [\bar{h}_{f,298}^{o} + (\bar{h}_{1000} - \bar{h}_{f,298}^{o})]_i$$

$$\bar{h}_{mix} = (x\bar{h}_i)_{CO} + (x\bar{h}_i)_{CO_2} + (x\bar{h}_i)_{H_2O} + (x\bar{h}_i)_{N_2} + (x\bar{h}_i)_{NO}$$

$$\bar{h}_{mix} = 0.002[-110541 + 21697] + 0.127[-393546 + 33425] + 0.149[-241847 + 25993]$$
$$+ 0.722[0 + 21468] + 106 \times 10^{-6}[90297 + 22241]$$

$$\boxed{\bar{h}_{mix} = -62563 \ ^{KJ}/_{kmole}}$$

COMMENTS: Note how much the N_2 contributes to the mixture specific enthalpy (15500 $^{KJ}/_{kmole-mix}$) despite having a relatively small absolute enthalpy itself (21468 $^{KJ}/_{kmole-N_2}$). This is due to the large mole fraction of N_2 present in the mixture.

PROBLEM 2-25

GIVEN: Methane lower heating value, $LHV = 50,016 \ \frac{KJ}{Kg}\text{-fuel}$ at 298 K

FIND: The lower heating value per:
    a) mass of fuel-air mixture
    b) Kmole of fuel-air mixture
    c) cubic meter of fuel-air mixture

ASSUMPTIONS: fuel-air mixture behaves as an ideal gas and P=1atm

APPROACH: Determine the stoichiometric A/F ratio for methane and using this mixture ratio perform a units conversion

Stoichiometric relation: $CH_4 + aO_2 + 3.76a \, N_2 \rightarrow CO_2 + 2H_2O + 3.76a \, N_2$

$$\text{for } \phi = 1 \quad a = x + y/4 \quad x=1 \quad y=4$$
$$a = 2$$

a) $\quad \left(\frac{A}{F}\right)_{MASS} = 4.76a \, \frac{MW_{air}}{MW_{fuel}} = 4.76(2) \frac{28.85}{16.043} = 17.12 \ \frac{Kg\text{-air}}{Kg\text{-fuel}}$

$$LHV \left[\frac{KJ}{Kg\text{-mix}} \right] = LHV \left[\frac{KJ}{Kg\text{-fuel}} \right] \left(\frac{1}{1 + A/F} \right) \left[\frac{Kg\text{-fuel}}{Kg\text{-mix}} \right]$$

$$LHV \left[\frac{KJ}{Kg\text{-mix}} \right] = \left(50016 \ \frac{KJ}{Kg\text{-f}} \right) \left(\frac{1}{1+17.12} \ \frac{Kg\text{-fuel}}{Kg\text{-mix}} \right)$$

$$\boxed{LHV = 2760 \ \frac{KJ}{Kg\text{-mix}}}$$

b) $\quad \left(\frac{A}{F}\right)_{MOLAR} = 4.76a = 4.76(2) = 9.52 \ \frac{Kmol\text{-air}}{Kmol\text{-fuel}}$

$$LHV \left[\frac{KJ}{Kmol\text{-mix}} \right] = LHV \left[\frac{KJ}{Kg\text{-fuel}} \right] \cdot MW_f \left[\frac{Kg\text{-fuel}}{Kmole\text{-fuel}} \right] \cdot \frac{1}{1 + A/F} \left[\frac{KMOL\text{-fuel}}{KMOL\text{-mix}} \right]$$

$$LHV \left[\frac{KJ}{Kmol\text{-mix}} \right] = (50016)(16.043) \left(\frac{1}{1 + 9.52} \right) = 76274 \ \frac{KJ}{Kmole\text{-mix}}$$

$$\boxed{LHV \left[KJ/Kmol\text{-mix} \right] = 76274 \ \frac{KJ}{Kmole\text{-mix}}}$$

c) $\quad LHV \left[KJ/m^3\text{-mix} \right] = LHV \left[\frac{KJ}{KMOL\text{-MIX}} \right] \cdot \frac{N}{V} \left(\frac{Kmol\text{-mix}}{m^3} \right)$

Assuming ideal gas $\quad \frac{N}{V} = \frac{P}{R_u T} = \frac{101.325}{(8.315)(298)} = 0.0409 \ \frac{KMOLS}{m^3}$

$$LHV \left[KJ/m^3\text{-mix} \right] = \left(76274 \ \frac{KJ}{Kmol} \right) \left(0.0409 \ \frac{KMOLS}{m^3} \right) = 3119 \ \frac{KJ}{m^3\text{-mix}}$$

$$\boxed{LHV \left[KJ/m^3\text{-mix} \right] = 3119 \ \frac{KJ}{m^3\text{-mix}}}$$

GIVEN: The higher heating value of liquid octane (C_8H_{18}) at 298 K is 47893 KJ/kg-f and the enthalpy of vaporization is 363 KJ/kg-fuel

FIND: The enthalpy of formation of ocatane vapor at 298 K

ASSUMPTIONS: Complete combustion, all H_2O exists in liquid form, and no dissociation

APPROACH: Determine the product composition for stoichiometric combustion of octane. Then use a first law analysis to calculate the enthalpy of formation for liquid octane, from which the vapor enthalpy can be found.

Stoichiometric relation:

$$C_8H_{18} + aO_2 + 3.76aN_2 \longrightarrow 8CO_2 + 9H_2O_{(\ell)} + 3.76aN_2$$
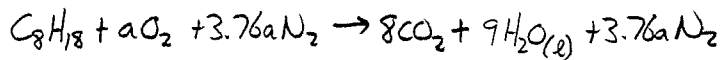
Since the reactants and products are at 298 K, the sensible enthalpies of all species are zero and the O_2 and N_2 heats of formation are zero. Consequently O_2 and N_2 can be neglected in this calculation.

$Q = HHV$

H_R $T = 298K$

H_P $T = 298K$
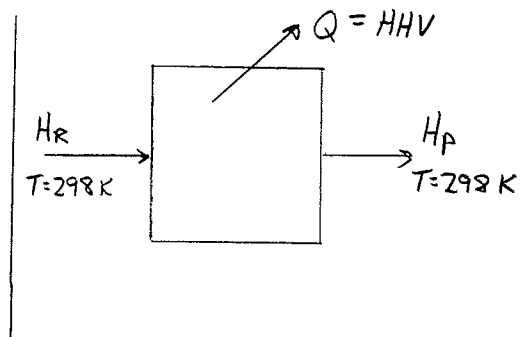
first law analysis: $H_{R,298} = H_P + HHV$ at steady-state

$$H_{P,298} = 8\left[\bar{h}_f^\circ\right]_{CO_2} + 9\left[\bar{h}_{f_{H_2O(v)}}^\circ - \bar{h}_{fg,H_2O}\right]_{H_2O(\ell)} = 8\left[-393546\right]_{CO_2} + 9\left[-241847 - 44011\right]_{H_2O(\ell)}$$

$$H_{P,298} = -5.7211 \times 10^6 \text{ KJ} \qquad \text{(enthalpies from appendix A)}$$

$$H_{R,298} = (1)\left[\bar{h}_f^\circ\right]_{C_8H_{18}(\ell)}$$

$$HHV\left[KJ/kmol\text{-fuel}\right] = HHV\left[KJ/kg\text{-f}\right] MW_{fuel}\left[\frac{kg\text{-f}}{kmol\text{-f}}\right] = 47893(114.23) = 5.471 \times 10^6 \text{ } KJ/kmol\text{-f}$$

$$H_{R,298} = H_{P,298} + HHV(1 \text{ kmol-fuel}) \longrightarrow \bar{h}_{f_{C_8H_{18}(\ell)}}^\circ = -5.7211 \times 10^6 + 5.471 \times 10^6 \text{ } KJ/kmol$$
$$= -250273 \text{ } KJ/kmol\text{-fuel}$$

$$\bar{h}_{f_{C_8H_{18}(v)}}^\circ = \bar{h}_{f_{C_8H_{18}(\ell)}}^\circ + h_{fg_{C_8H_{18}}} = -250273 \text{ } KJ/kmol\text{-f} + 363 \text{ } KJ/kg\text{-f}\left[114.23 \frac{kg\text{-f}}{kmol}\right]$$

$$\boxed{\bar{h}_{f_{C_8H_{18}(v)}}^\circ = -208807 \text{ } KJ/kmol}$$

COMMENTS: The absolute enthalpy of a species in the vapor-phase can be found from the liquid-phase enthalpy:
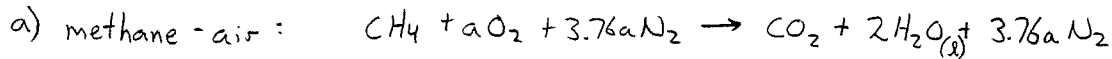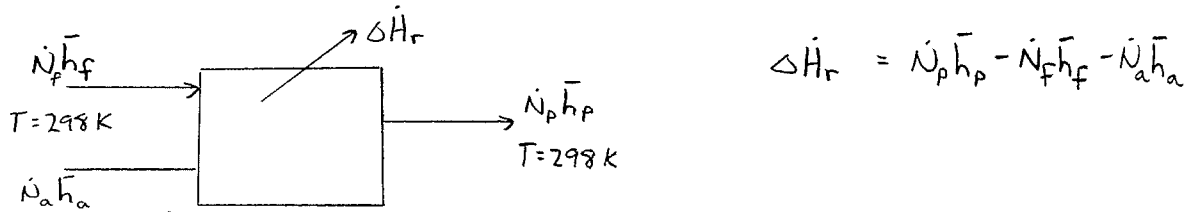Results agree well with appendix B.1

$$h_{(v)} = h_{(\ell)} + h_{fg}$$

GIVEN: The following reactions : CH_4-air , H_2-O_2 , and $C(s)$ -air

FIND: the heat of reaction Δh_r in KJ/kg-fuel , KJ/kg-mix and the A/F (mass) ratio. Compare the results with table 2.1.

ASSUMPTIONS: complete combustion , no species dissociation

APPROACH: Calculate the A/F ratio using conservation of elements and then determine Δh_r from the first law of thermodynamics.

$$\Delta \dot{H}_r = \dot{N}_p \bar{h}_p - \dot{N}_f \bar{h}_f - \dot{N}_a \bar{h}_a$$

a) methane - air : $CH_4 + aO_2 + 3.76aN_2 \rightarrow CO_2 + 2H_2O_{(\ell)} + 3.76aN_2$

$$a = \frac{x+y/4}{\phi} = 2 \quad \text{for} \quad x=1, y=4, \phi=1$$

$$\boxed{A/F = 4.76a\left(\frac{MW_a}{MW_f}\right) = 4.76(2)\left(\frac{28.85}{16.043}\right) = 17.12}$$

first law : $\Delta \bar{h}_r = \dfrac{\Delta \dot{H}_r}{\dot{N}_f} = \sum \dfrac{\dot{N}_i}{\dot{N}_f} \bar{h}_{i,p} - \bar{h}_f - a\bar{h}_{O_2} - 3.76a\bar{h}_{N_2}$

$\Delta \bar{h}_r = 1 \left[-393546\right]_{CO_2} + 2\left[-285856\right]_{H_2O(\ell)} - \left[-74831\right] - 2\left[0\right]_{O_2} - 7.52\left[0\right]_{O_2}$

for products and reactants at 298 K (i.e., $\bar{h} = \bar{h}_f^{\circ}$)

$\Delta \bar{h}_r = -890.427 \; KJ/kmol$-f $\longrightarrow \Delta h_r \left[KJ/kg\text{-}f\right] = \Delta \bar{h}_r \left[KJ/kmole\text{-}f\right] \cdot \dfrac{1}{MW_f} \left[\dfrac{kmole\text{-}f}{kg\text{-}f}\right]$

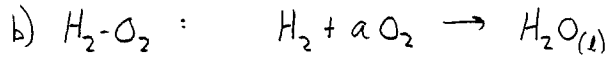$$\boxed{\Delta h_r = -890427\left(\frac{1}{16.043}\right) = -55503 \; KJ/kg\text{-}f}$$

$\Delta h_r \left[KJ/kg\text{-}mix\right] = \Delta h_r \left[KJ/kg\text{-}f\right] \cdot \dfrac{1}{1+A/F} \left[\dfrac{kg\text{-}F}{kg\text{-}mix}\right]$

$\Delta h_r \left[KJ/kg\text{-}mix\right] = -55503 \cdot \dfrac{1}{1+17.12}$

$$\boxed{\Delta h_r = -3063 \; KJ/kg\text{-}mix}$$

(continued)

b) $H_2 - O_2$: $H_2 + aO_2 \longrightarrow H_2O_{(\ell)}$

$$a = \frac{x + y/4}{\phi} = \frac{1}{2} \qquad \text{for} \quad x = 0, \ y = 2, \ \phi = 1$$

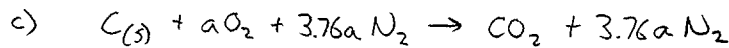$$A/F = a \frac{MW_{O_2}}{MW_{H_2}} = \frac{1}{2}\left(\frac{32}{2}\right) = 8 \qquad \boxed{A/F = 8}$$

$$\Delta\bar{h}_r = \sum \frac{N_i}{N_f} \bar{h}_{P,i} - a\bar{h}_{O_2} - \bar{h}_f = 1\,\bar{h}_{H_2O(\ell)} - 2\,\bar{h}_{O_2} - \bar{h}_{H_2}$$

$$= 1[-285856] - 2[0] - 1[0]$$

$$\Delta\bar{h}_r = -285856 \ ^{KJ}/_{Kmole-f}$$

$$\Delta h_r = \Delta\bar{h}_r \cdot \frac{1}{MW_f} = -\frac{285856}{2} \longrightarrow \boxed{\Delta h_r = -142928 \ ^{KJ}/_{Kg-f}}$$

$$\Delta h_r \left[^{KJ}/_{Kg-mix}\right] = \Delta h_r \left[^{KJ}/_{Kg-f}\right] \cdot \frac{1}{1 + A/F} = -142928\left(\frac{1}{1+8}\right)$$

$$\boxed{\Delta h_r \left[^{KJ}/_{Kg-mix}\right] = -15880 \ ^{KJ}/_{Kg-mix}}$$

c) $C_{(s)} + aO_2 + 3.76a\,N_2 \longrightarrow CO_2 + 3.76a\,N_2$

$$a = \frac{x + y/4}{\phi} = 1 \quad \text{for } x=1, y=0, \phi=1 \qquad A/F = 4.76a\left(\frac{MW_a}{MW_f}\right) = 4.76(1)\left(\frac{28.85}{12}\right)$$

$$\boxed{A/F = 11.44}$$

$$\Delta\bar{h}_r = \sum \frac{N_i}{N_f} \bar{h}_{P,i} - a\bar{h}_{O_2} - 3.76a\bar{h}_{N_2} - \bar{h}_f = 1[-393546]_{CO_2} - 1[0]_{O_2} - 3.76[0]_{N_2} - 1[0]_{C(s)}$$

$$\Delta\bar{h}_r = -393546 \ ^{KJ}/_{Kmole-f}$$

$$\Delta h_r \left[^{KJ}/_{Kg-f}\right] = \Delta\bar{h}_r \cdot \frac{1}{MW_f} = -393546 \cdot \frac{1}{12} = -32796 \ ^{KJ}/_{Kg-f} \qquad \boxed{\Delta h_r = -32796 \ ^{KJ}/_{Kg-f}}$$

$$\Delta h_r \left[^{KJ}/_{Kg-mix}\right] = \Delta h_r \left[^{KJ}/_{Kg-f}\right] \frac{1}{1 + A/F} = -32796\left(\frac{1}{1 + 11.44}\right) = -2636 \ ^{KJ}/_{Kg-mix} \qquad \boxed{\Delta h_r = -2636 \ ^{KJ}/_{Kg-mix}}$$

GIVEN: A stoichiometric mixture of propane (C_3H_8) and air

FIND: Δh_r $(kJ/kg\text{-}f)$, Δh_r $(kJ/kg\text{-}mix)$, and A/F (mass) ratio

ASSUMPTIONS: Complete combustion with no dissociation, water in combustion products exists in liquid-phase since $T = 298\,K$

APPROACH: Calculate the A/F ratio using elemental conservation and then determine Δh_r from the first law of thermodynamics

combustion equation:

$$C_3H_8 + aO_2 + 3.76aN_2 \longrightarrow 3CO_2 + 4H_2O + 3.76aN_2$$

$$a = \frac{x + y/4}{\phi} = \frac{3 + 2}{1} = 5 \longrightarrow A/F = 4.76a\,\frac{MW_{air}}{MW_{fuel}}$$

$$\boxed{A/F = 4.76(5)\left(\frac{28.85}{44}\right) = 15.57}$$

first law analysis:
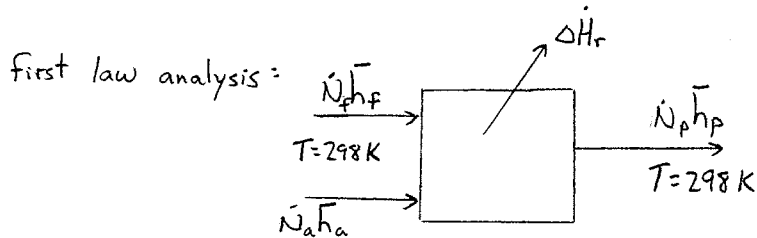
$$\Delta \dot{H}_r = \dot{H}_P - \dot{H}_R = \dot{N}_p \overline{h}_p - \dot{N}_a \overline{h}_a - \dot{N}_f \overline{h}_f \qquad \text{Note: at 298 K } \overline{h} = \overline{h}_f^\circ + \cancelto{0}{(\overline{h} - \overline{h}_f^\circ)}$$

$$\Delta \overline{h}_r = \frac{\Delta \dot{H}_r}{\dot{N}_f} = \Sigma \frac{\dot{N}_i}{\dot{N}_f} \overline{h}_{P,i} - a\cancelto{0}{\overline{h}_{O_2}} - 3.76a\cancelto{0}{\overline{h}_{N_2}} - \overline{h}_f$$

$$\Delta \overline{h}_r = 3\overline{h}_{f\,CO_2}^\circ + 4\overline{h}_{f, H_2O(\ell)}^\circ - \overline{h}_{f, f}^\circ = 3[-393546] + 4[-285856] - [-103847]$$

$$\Delta \overline{h}_r = -2.2202 \times 10^6 \; kJ/kmole\text{-}f$$

$$\Delta h\,[kJ/kg\text{-}fuel] = \Delta \overline{h}_r\,(kJ/kmole) \cdot \frac{1}{MW_f}\left[\frac{kmole}{kg\text{-}f}\right] = -2.2202 \times 10^6 \left[\frac{1}{44.096}\right]$$

$$\boxed{\Delta h_r = -50349 \; kJ/kg\text{-}f}$$

$$\Delta h_r\,\left[kJ/kg\text{-}mix\right] = \Delta h_r\,\left[kJ/kg\text{-}f\right] \cdot \frac{1}{1 + A/F}\left[\frac{kg\text{-}f}{kg\text{-}mix}\right] = -50459\left(\frac{1}{1+15.57}\right)$$

$$\boxed{\Delta h_r = -3039 \; kJ/kg\text{-}mix}$$

COMMENTS: Note that this Δh_r is based on condensed H_2O in the product mixture. Also, $\Delta h_r\,(kJ/kg\text{-}f) = -HHV$ from Appendix B.1 as would be expected.

GIVEN: A liquid fuel undergoing combustion

FIND: On an h-T sketch illustrate the following quantities; $h_\ell(T)$, $h_v(T)$, enthalpy of vaporization, h_{fg}, enthalpy of formation for fuel vapor, enthalpy of formation for fuel liquid, lower heating value, and higher heating value
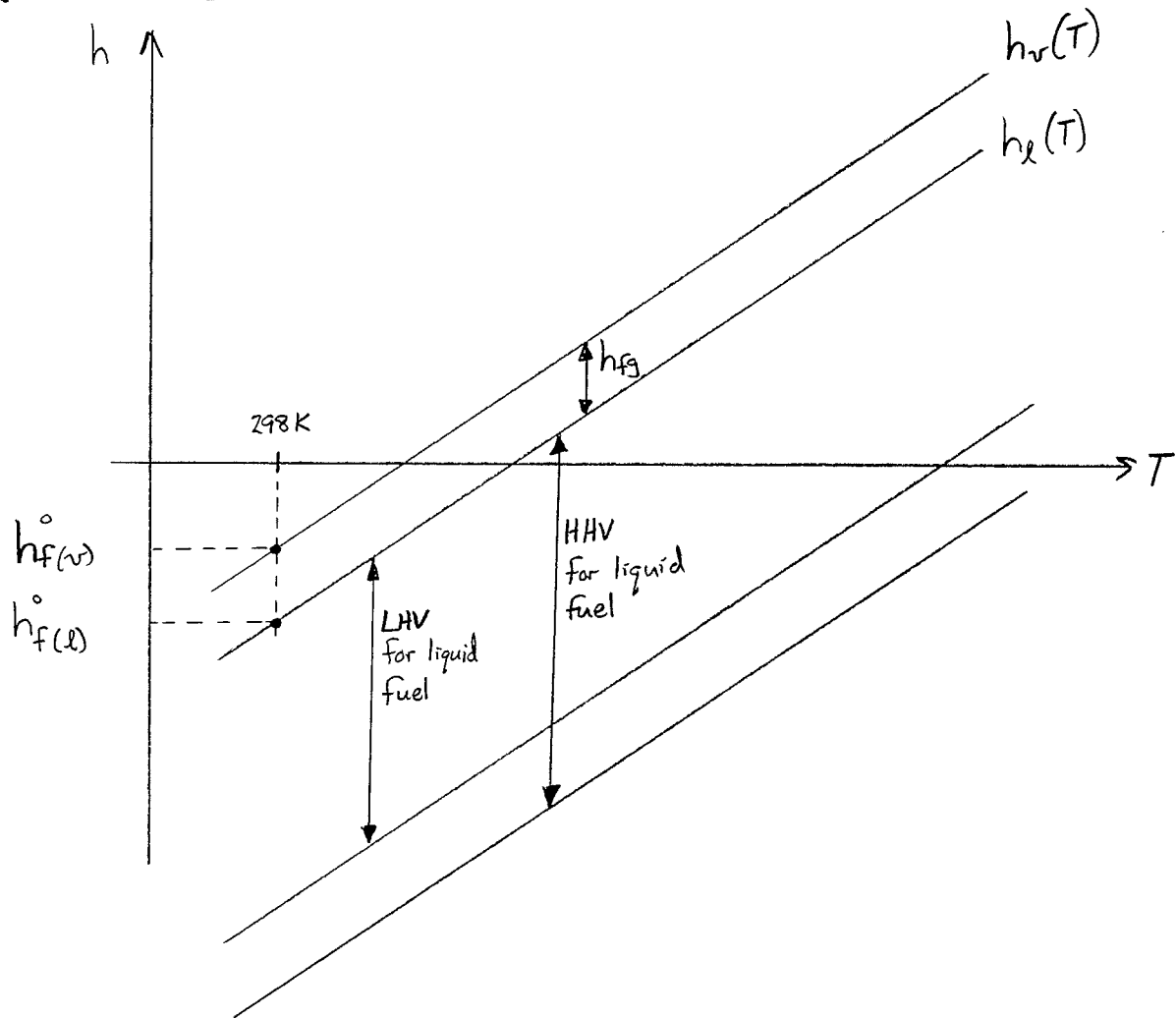
COMMENTS: Note that the greatest enthalpy change at T=const (or greatest temperature change for h=const) occurs when fuel vapor is burned and the products contain liquid H_2O. Also, the lower and higher heating values for fuel vapor can be found by adding the enthalpy of vaporization to the fuel liquid lower and higher heating values.
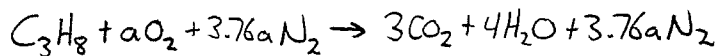
GIVEN: A stoichiometric propane (C_3H_8)-air mixture at 298 K

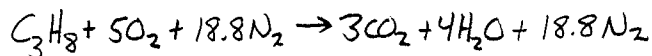FIND: The adiabatic flame temperature, T_{ad}

ASSUMPTIONS: no dissociation, constant specific heats evaluated at 298 K

APPROACH: Use element conservation to determine the correct fuel-air mix and product composition. Then use a first law analysis to evaluate T_{ad}

Stoichiometric relation:
$$C_3H_8 + aO_2 + 3.76aN_2 \rightarrow 3CO_2 + 4H_2O + 3.76aN_2$$

$$at \quad \phi=1 \quad a = x + Y/4 = 5$$

$$C_3H_8 + 5O_2 + 18.8N_2 \rightarrow 3CO_2 + 4H_2O + 18.8N_2$$

(Since the reactants are at $T=298K$ the O_2 and N_2 contributions to the reactant enthalpy are zero)

H_R → [CV] → H_P
$T=298K$ $T=T_{ad}$
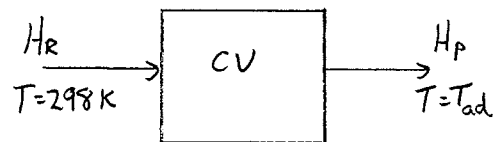
first law for adiabatic conditions: $H_{R_{298}} = H_{P_{T_{ad}}}$

$$[N\bar{h}]_{C_3H_8} + [N\bar{h}]_{O_2}^{0} + [N\bar{h}]_{N_2}^{0} = [N\bar{h}]_{CO_2} + [N\bar{h}]_{H_2O} + [N\bar{h}]_{N_2}$$

where $\bar{h} = \bar{h}_f^o + (\bar{h} - \bar{h}_{f,298}^o) = \bar{h}_f^o + \bar{c}_p(T-298)$ ← properties from appendix A

(1) $[-103847 + 0]_{C_3H_8} = 3[-393546 + 37.198(T_{ad}-298)]_{CO_2} + 4[-241847 + 33.448(T_{ad}-298)]_{H_2O}$

$$+ 18.8[0 + 29.071(T_{ad}-298)]_{N_2}$$

Solving for T_{ad}: $\boxed{T_{ad} = 2879 \ K}$

COMMENTS: Note that this flame temperature is much greater than the adiabatic flame temperature in appendix B.1. This is due to the assumption of no species dissociation and the assumption of constant specific heats evaluated at 298K. An examination of appendix A shows that the specific heats can vary significantly from 298 K to 2879 K.

PROBLEM 2-31

GIVEN: A stoichiometric propane (C_3H_8)-air mixture at 298 K

FIND: The adiabatic flame temperature, T_{ad}

ASSUMPTIONS: no dissociation, constant specific heats evaluated at 2000 K

APPROACH: Use element conservation to determine the correct fuel-air mixture and product composition. Then use a first law analysis to evaluate T_{ad}
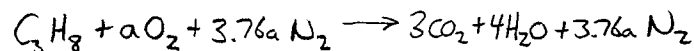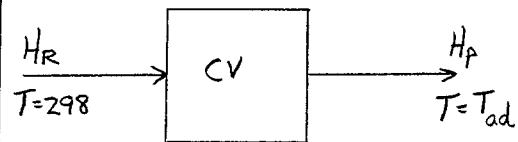
Stoichiometric relation:
$$C_3H_8 + aO_2 + 3.76a\,N_2 \longrightarrow 3CO_2 + 4H_2O + 3.76a\,N_2$$

at $\phi = 1$ $a = x + y/4 = 5$

$$C_3H_8 + 5O_2 + 18.8N_2 \longrightarrow 3CO_2 + 4H_2O + 18.8N_2$$

(Since the reactants are at $T = 298\,K$ the O_2 and N_2 contributions to the reactant enthalpy are zero)

first law for adiabatic conditions: $H_{R_{298}} = H_{P_{T_{ad}}}$

$$[N\bar{h}]_{C_3H_8} + [N\cancel{\bar{h}}]_{O_2}^{0} + [N\cancel{\bar{h}}]_{N_2}^{0} = [N\bar{h}]_{CO_2} + [N\bar{h}]_{H_2O} + [N\bar{h}]_{N_2}$$

where $\bar{h} = \bar{h}^{\circ}_{f,298} + (\bar{h} - \bar{h}^{\circ}_{f,298}) = \bar{h}^{\circ}_f + C_p(T - 298)$ ⟵ $\bar{h}^{\circ}_f$ and C_p from appendix A

$$(1)\ [-103847 + 0]_{C_3H_8} = 3[-393546 + 60.433(T_{ad} - 298)]_{CO_2} + 4[-241847 + 51.143(T_{ad} - 298)]_{H_2O}$$
$$+ 18.8[0 + 35.988(T_{ad} - 298)]_{N_2}$$

Solving for T_{ad}: $\boxed{T_{ad} = 2222\ K}$

COMMENTS: Note that this flame temperature is much closer to the value listed in appendix B.1 than the temperature calculated in problem 2-17. This is due to a more appropriate estimate of the constant specific heats. The effects of dissociation on the flame temperature are still unaccounted for.

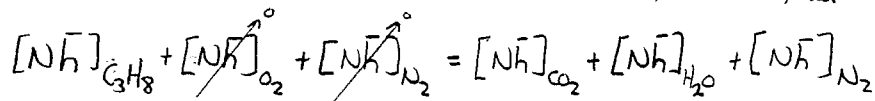GIVEN: A stoichiometric propane (C_3H_8)-air mixture

FIND: The adiabatic flame temperature, T_{ad}

ASSUMPTIONS: no dissociation, species thermophysical properties equal to those in appendix A

APPROACH: Use element conservation to determine the correct fuel-air mixture and product composition. Then use appendix A to evaluate the species thermophysical properties and a first law analysis to determine the flame temperature. This is an iterative process in which a flame temperature is guessed, the first law is checked, and if necessary a new flame temperature is chosen.

See problems 2-17 and 2-18 for correct fuel-air mixture and product composition. A control volume sketch for the energy conservation is also shown

first law for adiabatic conditions: $H_{R,298} = H_{P,T_{ad}} \longrightarrow H_P - H_R = 0$

$$[N\bar{h}]_{C_3H_8} + [N\bar{h}]^o_{O_2} + [N\bar{h}]^o_{N_2} = [N\bar{h}]_{CO_2} + [N\bar{h}]_{H_2O} + [N\bar{h}]_{N_2}$$

where $\bar{h} = \bar{h}^o_{f_{298}} + (\bar{h} - \bar{h}^o_{f,298}) = \bar{h}^o_f + \Delta h_s$ $\longleftarrow$ values from appendix A

(1) $[-103847] = 3[-393546 + \Delta h_s]_{CO_2} + 4[-241847 + \Delta h_s]_{H_2O} + 18.8[0 + \Delta h_s]_{N_2}$

Rearranging in form $H_P - H_R = 0$: $3\Delta h_{s,CO_2} + 4\Delta h_{s,H_2O} + 18.8\Delta h_{s,N_2} - 2.0442 \times 10^6 = 0$

T (K)	$\Delta h_{s,CO_2}$ (KJ/KMOL)	$\Delta h_{s,H_2O}$ (KJ/KMOLE)	$\Delta h_{s,N_2}$ (KJ/KMOLE)	$H_P - H_R$
2000	91420	72805	56130	-423476
2100	97477	77952	59738	-316887
2200	103562	83160	63360	-209706
2300	109670	88426	66997	-161942
2400	115798	93744	70645	6296

LINEAR INTERPOLATION USING $H_P - H_R = 0$

$$\boxed{T_{ad} = 2394 \text{ K}}$$

Comments: Note that this flame temperature is slightly greater than that listed in appendix B.1 despite using accurate thermophysical properties from appendix A. This is due to neglecting species dissociation.

GIVEN: A stoichiometric propane (C_3H_8)-mixture at 298 K

FIND: The adiabatic flame temperature using the computer code HPFLAME or other software. Compare and contrast the results of problems 2-17 to 2-20

Using HPFLAME: $\boxed{T_{ad} = 2267 \text{ K}}$ which matches appendix B.1

The adiabatic flame temperatures calculated in problems 2-17 through 2-20 differ for two main reasons; the method of evaluating the thermophysical properties and whether dissociation of the product species is considered. In problem 2-17 the species sensible enthalpies were estimated using constant specific heats at 298 K. Thus, $\Delta h_{sens} = \int_{298}^{T_{ad}} C_p \, dT \longrightarrow \Delta h_{sens} = C_{p,298} (T_{ad} - 298)$.

Since specific heat increases with temperature, we were effectively using too low of a specific heat, resulting in too high of an adiabatic flame temperature for a given Δh_{sens}.

In problem 2-18 the adiabatic flame temperature was calculated using constant specific heats evaluated at 2000 K. While using these specific heats yields an adiabatic flame temperature close to that listed in appendix B.1, the thermophysical properties are wrong. This can be seen by comparing the adiabatic flame temperature calculated in problem 2-18 (above) with that calculated in problem 2-19. In problem 2-19, tabulated values of sensible enthalpies (Appendix A) were used but the calculated flame temperature is much greater than that calculated using HPFLAME or listed in appendix B.1. This difference can not be attributed to incorrect thermophysical properties and must therefore be due to dissociation of the product species.

From the results of problems 2-17 through 2-20 it becomes apparent that accurate evaluation of mixture thermophysical properties and product dissociation are required to obtain a close calculation of adiabatic flame temperature.

GIVEN: Equimolar fuel blend of C_3H_8 & CH_4 burns in air ($\Phi = 0.8$)

$$T_{air} = T_F = 298K$$
$$P = 1\,atm = constant$$

FIND: T_{ad}
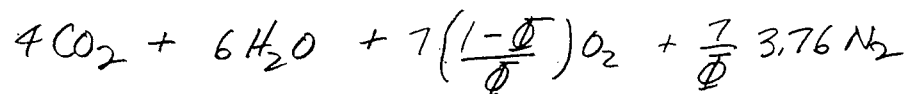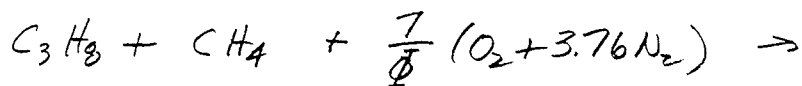
ASSUMPTIONS: No dissociation (given)
Constant $\bar{c}_p$ @ 1200K (given)
Air = 79% N_2, 21% O_2

SOLUTION: Apply 1st-law, Eqn 2.40a:

$$H_R (T_i, P) = H_{Pr} (T_{ad}, P)$$

To evaluate the above, we need to determine the composition of the reactants and products:

$$C_3H_8 + CH_4 + \frac{7}{\Phi} (O_2 + 3.76N_2) \rightarrow$$

$$4CO_2 + 6H_2O + 7\left(\frac{1-\Phi}{\Phi}\right)O_2 + \frac{7}{\Phi}3.76N_2$$

Reactants:

	N	$\bar{h}\,(=\bar{h}_f^o)$	$N\bar{h}$	Table
C_3H_8	1	−103,847	−103,847	B.1
CH_4	1	−74,831	−74,831	B.1
O_2	8.75	0	0	—
N_2	32.90	0	0	—

$$H_R = \sum N_i \bar{h}_i = -178,678 \; [=] \; kJ$$

Products:

	N	$\bar{h}_f^o$	$\bar{c}_p$ @ 1200K	$N\bar{h}_f^o$	$N\bar{c}_p$	Table
CO_2	4	$-393,546$	54.360	$-1,574,184$	217.440	A.2
H_2O	6	$-291,845$	43.874	$-1,451,070$	263.244	A.6
O_2	1.75	0	34.936	0	61.138	A.11
N_2	32.90	0	32.762	0	1077.870	A.7
				$-3,025,254$	1619.692	

$$H_{Pr} = \sum N_i \bar{h}_i = \sum N_i \left[\bar{h}_{f_i}^o + \bar{c}_{p_i} (T_{ad} - 298.15) \right]$$

$$= \sum N_i \bar{h}_{f_i} + \sum N_i \bar{c}_{p_i} (T_{ad} - 298.15)$$

$$H_{Pr} = -3,025,254 + 1619.692 (T_{ad} - 298.15) \, [=] \, kJ$$

$$H_R = H_P \quad (Eqn. \ 2.40a)$$

$$-178,678 = -3,025,254 + 1619.692 (T_{ad} - 298.15)$$

$$T_{ad} - 298.15 = \frac{-178,678 + 3,025,254}{1619.692} = 1978.1$$

$$\boxed{T_{ad}} = 1978.1 + 298.15 = \boxed{2276 \ K}$$

COMMENTS: Tabulating needed information for reactants & products helps to organize calculations of this type.

GIVEN: C_3H_8 - air

$\Phi = 1$, $T_i = 298$, $P_i = 1\,atm$
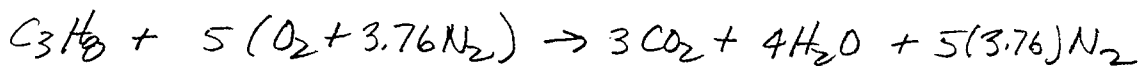
constant-volume combustion

FIND: T_{ad}, P_{final}

ASSUMPTIONS: No dissociation (given)

Constant $\bar{c}_{p,i}$ @ 298 K

Air $\equiv$ 79% N_2, 21% O_2

SOLUTION: Apply 1st law, Eqn. 2.41:

$$\bar{U}_R (T_i, P_i) = \bar{U}_{Pr} (T_{ad}, P_f)$$

or

$$H_R - H_{Pr} - R_u (N_R T_i - N_{Pr} T_{ad}) = 0 \qquad Eqn.\ 2.43$$

To evaluate Eqn. 2.43, we need the composition of both the reactants & products:

$$C_3H_8 + 5(O_2 + 3.76 N_2) \rightarrow 3CO_2 + 4H_2O + 5(3.76)N_2$$

Reactants:

	N	$\bar{h}(=\bar{h}_f^{\circ})$	$N\bar{h}$	Table
C_3H_8	1	$-103,847$	$-103,847$	B.1
O_2	5	0	0	—
N_2	18.8	0	0	—
$\sum_R$	24.8 kmol		$-103,847$ kJ	

$$H_R = \sum_R N_i h_i = -103,847 \text{ kJ}$$

Products:

	N	$\bar{h}_f^o$	$\bar{c}_p$ @ 298K	$N\bar{h}_f^o$	$N\bar{c}_p$	Table
CO_2	3	−393,546	37.198	−1,180,638	111.594	A.2
H_2O	4	−241,845	33.448	−967,380	133.792	A.6
N_2	18.8	0	29.071	0	546.535	A.7
$\sum_{Pr}$	25.8			−2,148,018	791.921	

$$H_{pr} = \sum_{Pr} N_i \bar{h}_i = \sum N_i \left[\bar{h}_{f_i} + \bar{c}_{p,i} (T_{ad} - T_{ref}) \right]$$

$$= \sum N_i \bar{h}_{f_i} + \sum N_i \bar{c}_{p_i} (T_{ad} - T_{ref})$$

$$H_{pr} = -2,148,018 + 791.921 (T_{ad} - T_{ref})$$

Substituting into Eqn. 2.43 with $T_{ref} = T_i$,

$$H_R - H_{pr} - R_u N_R T_i + R_u N_{pr} T_{ad} = 0$$

$$-103,847 - \left[-2,148,018 + 791.921 (T_{ad} - T_i) \right]$$

$$- 8.3145 (24.8) 298.15 + 8.3145 (25.8) T_{ad} = 0$$

Simplifying:

$$2,218,804 - 577.407 \; T_{ad} = 0$$

$$\boxed{T_{ad} = 3843 \; K}$$

$$\forall = \frac{N_R R_u T_i}{P_i} = \frac{N_{pr} R_u T_{ad}}{P_f} \Rightarrow P_f = P_i \frac{N_{pr}}{N_r} \frac{T_{ad}}{T_i}$$

$$\boxed{P_f =} 1 \, atm \; \frac{25.8}{24.8} \; \frac{3843}{298.15} = \boxed{13.4 \, atm}$$

COMMENT: As expected, the constant-vol. adia. flame temperature is significantly greater than the const.-P value of 2879 K from Problem 2.30.
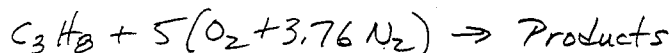
GIVEN: C_3H_8 - air ; $\underline{\Phi} = 1$; $T_i = 298\,K$; $P_i = 1\,atm$.

FIND: T_{ad} @ constant volume , P_{final}

ASSUMPTIONS: Ideal gas ; product dissociation .

SOLUTION: To use UVFLAME, we need to determine
H_R (per kmol of fuel), N_R, and MW_R :

$$C_3H_8 + 5(O_2 + 3.76\,N_2) \Rightarrow \text{Products}$$

$$H_R = (1)\left[\bar{h}^{\circ}_{f,C_3H_8} + \cancel{\Delta \bar{h}_{s,C_3H_8}}^{0}\right] + 5\left[\bar{h}^{\circ}_{f,O_2} + \cancel{\Delta \bar{h}_{s,O_2}}^{0}\right] + 5(3.76)\left[\cancel{\bar{h}^{\circ}_{f,N_2}}^{0} + \cancel{\Delta \bar{h}_{s,N_2}}^{0}\right]$$

$$H_R = -103,848 \;\; kJ/kmol_{C_3H_8} \quad (\text{Table B.1})$$

$$N_R = 1 + 5(4.76) = 24.8 \; kmol$$

$$MW_R = \frac{(1)\,44.096 + 23.8(28.85)}{24.8} = 29.465$$

OUTPUT FROM UVFLAME:

```
Constant-Volume Adiabatic Flame Calculation for Specified Fuel,
Phi, & Reactant Properties Using Olikara & Borman Equilibrium Routines


Problem Title: PROBLEM 2.36 (2nd Ed.)

 Data below are as read from the input file.
 Compare with INPUT.UV. If they do not agree, your
 input data have not been entered correctly.

 CARBON ATOMS                            3.0
 HYDROGEN ATOMS                          8.0
 OXYGEN ATOMS                            0.0
 NITROGEN ATOMS                          0.0
 EQUIVALENCE RATIO                       1.000
 FINAL TEMPERATURE (K) guess          2500.0
 REACTANT TEMPERATURE (K)              298.1
 REACTANT PRESSURE (Pa)                 101325.0
 ENTHALPY OF REACTANTS (kJ/kmol of fuel)   -103848.0
 MOLES OF REACTANTS (kmol/kmol of fuel)    24.800
 MOLEC WT OF REACTANTS (kg/kmol)           29.465
```

FLAME TEMP. & COMBUSTION PRODUCTS PROPERTIES

```
Const-vol Flame Temperature [K] =        2631.53
Pressure [Pa] =                          0.946107E+06
Mixture Enthalpy [J/kg] =                0.5593E+06
Mixture Specific Heat, Cp [J/kg-K] =     0.255109E+04
Specific Heat Ratio, Cp/Cv =             1.1531
Mixture Molecular Weight [kg/kmol] =     27.8520
Moles of Fuel per Mole of Products =     0.03809654
```

The mole fractions of the product species are:

```
H:   0.00104322   O:   0.00083162   N:   0.00000026
H2:  0.00538231   OH:  0.00664940   CO:  0.02220778
NO:  0.00594248   O2:  0.00910174   H2O: 0.14315753
CO2: 0.09208184   N2:  0.71360183
```

From above:

$$T_{ad} = 2631.5 \ K$$

$$P_{final} = 9.46107 \cdot 10^5 \ Pa \quad = 9.337 \ atm$$

Compared with results using c_p's evaluated at 298 K and ignoring dissociation (Problem 2.35), these values are much lower ($T_{ad} = 2632 \ K$ vs. 3843 K). This is as expected, since c_p's @ 298 K are much too low and dissociation is important.

COMMENT: Note the minimal computation required to use UVFLAME to calculate constant-volume adiabatic flame temperatures.