CombustionHelp.com HW1

***Question 1:***

Use stoichiometry to create balanced chemical reactions for the following fuels + air: methane, ethane, propane, butane, pentane, hexane, methyl decanoate (C11H22O2), unknown carbohydrate (CxHyOz)

***Answer 1:***

Methane is CH4

Starting Equation: CH4 + a\*O2 = b\*CO2 + c\*H2O

Balance C: 1 = b

Balance H: 4 = 2\*c

Balance O: 2\*a = 2\*b + c

Final Equation: CH4 + 2\*O2 = 1\*CO2 + 2\*H2O

Ethane is C2H6

Starting Equation: C2H6 + a\*O2 = b\*CO2 + c\*H2O

Balance C: 2 = b

Balance H: 6 = 2\*c

Balance O: 2\*a = 2\*b + c

Final Equation: CH4 + (7/2)\*O2 = 2\*CO2 + 3\*H2O

Propane is C3H8

Starting Equation: C3H8 + a\*O2 = b\*CO2 + c\*H2O

Balance C: 3 = b

Balance H: 8 = 2\*c

Balance O: 2\*a = 2\*b + c

Final Equation: CH4 + 5\*O2 = 3\*CO2 + 4\*H2O

Butane is C4H10

Starting Equation: C4H10 + a\*O2 = b\*CO2 + c\*H2O

Balance C: 4 = b

Balance H: 10 = 2\*c

Balance O: 2\*a = 2\*b + c

Final Equation: CH4 + (13/2)\*O2 = 4\*CO2 + 5\*H2O

Pentane is C5H12

Starting Equation: C5H12 + a\*O2 = b\*CO2 + c\*H2O

Balance C: 5 = b

Balance H: 12 = 2\*c

Balance O: 2\*a = 2\*b + c

Final Equation: CH4 + 8\*O2 = 5\*CO2 + 6\*H2O

Hexane is C6H14

Starting Equation: C6H14 + a\*O2 = b\*CO2 + c\*H2O

Balance C: 6 = b

Balance H: 14 = 2\*c

Balance O: 2\*a = 2\*b + c

Final Equation: CH4 + (19/2)\*O2 = 6\*CO2 + 7\*H2O

Methyl Decanoate is C11H22O2

Starting Equation: C11H22O2 + a\*O2 = b\*CO2 + c\*H2O

Balance C: 11 = b

Balance H: 22 = 2\*c

Balance O: 2+2\*a = 2\*b + c

Final Equation: CH4 + (31/2)\*O2 = 11\*CO2 + 11\*H2O

Unknown Carbohydrate is CxHyOz

Starting Equation: CxHyOz + a\*O2 = b\*CO2 + c\*H2O

Balance C: x = b

Balance H: y = 2\*c

Balance O: z+2\*a = 2\*b + c

Final Equation: CH4 + ()\*O2 = x\*CO2 + (y/2)\*H2O

***Question 2:***

Given hydrogen gas (H2) and air with “fuel-air equivalence ratio” phi = (1/2), calculate mole (X) and mass fractions (Y) of all product species, average molecular weight, and average specific heat () at P=1atm T=298.15K (standard state).

***Answer 2:***

Definition of “fuel-air equivalence ratio”

Where: m represents the mass, n represents number of moles, and suffix “st” stands for stoichiometric conditions.

Definition of mass fraction is:

Where N is the number of species and mi=Wi\*ni .

Definition of mole fraction is:

Air consists of 1 mole O2 for every 3.76 mole of N2 .

Molecular weight (W) of O2 is 32 kg/kmol, H2 is 2 kg/kmol, and N2 is 28 kg/kmol .

Note: specific heat, , is a function of both pressure and temperature.

(Also: , is a function of both specific volume and temperature.)

At T=298 K and P=1atm: of O2 =29.315 , of H2 =28.871 ,

and of N2 = 29.071

Where the line over indicates mole-based values.

The stoichiometric reaction for H2 and air is: 2\*H2 + O2 = 2\*H2O

Therefore

The mixture is 1 mole of H2, 1 mole of O2, 3.76 moles of N2 .

***Question 3:***

From the ideal gas law and first law of thermodynamics derive the isentropic relations for pressure and temperature.

***Answer 3:***

Ideal gas law: PV = nRuT V/m=v n=m/M R=

Where M is molecular weight of mixture in units kg/kmol .

Ru is universal gas constant with cgs units

Ideal gas law becomes: Pv=RT

Taking natural log of both sides: ln(P) + ln(v) = ln(R) + ln(T)

Taking derivative, that is multiplying equation by “d” (Note: d(ln R)=0 ):

d(ln P) + d(ln v) = d(ln T) [eq A]

First law of thermodynamics is conservation of energy

dU = dQ + dW dW=-PdV dU=cvdT dQ=TdS

Definition of isentropic: adiabatic (no heat transfer) and reversible process

Definition of reversible: process can be reversed with out dissipation of energy (entropy production), therefore there is no change in entropy of system.

Note relationship between specific heats and universal gas constant:

(mole based)

(mass based)

First law becomes (Note: TdS = 0 because reversible system):

Where we used the definition of natural log: =>

From this equation we solve for :

Substituting eq B into eq A, and manipulate, (note: heat capacity ratio, k=cp/cv) :

Using property of natural logs, we can move term:

Now integrate from state 1 to state 2:

Finally resulting in

***Question 4:***

From the ideal gas law and first law of thermodynamics derive the isentropic relations for pressure and specific volume.

***Answer 4:***

Substituting eq C into eq A of question 3, and manipulate:

Using property of natural logs, we can move term:

Now integrate from state 1 to state 2:

Finally resulting in

***Question 5:***

Derive the entropy change of ideal gases, using definitions of enthalpy (h=u+Pv) and entropy (ds=dq/T), first law of thermodynamics, and property relations for an ideal gas (ideal gas law, definitions of specific heats cp and cv)

If there is no temperature change this results in the following equations, where is the value of entropy at temperature T and standard state pressure P0:

Note: entropy changes can be expressed on a unit-mole basis by multiplying by molecular weight of mixture (Mmix has units of kg/kmol):

If there is no temperature change this results in the following equations, where is the value of entropy at temperature T and standard state pressure P0:

***Answer 5:***

Definition of first law of thermodynamics

Solving for ds:

Substitute du=cvdT and P=RT/v :

Integrate between state 1 and state 2, to obtain

Now to find equation with pressure instead of specific volume, start with definition of enthalpy:

And differentiate:

Substitute first law of thermodynamics and solve for ds:

Substitute dh=cpdT and v=RT/P :

Integrate between state 1 and state 2, to obtain

Additional note: the terms or can be simplified by assuming a constant average cv or cp value.