Quiz 4 Thermodynamics
February 6, 2020

Coal gasification is a process to convert solid fuel (coal) into a gas or liquid fuel. The original process resulted in the syngas "town gas" which was used as the first piped gaseous fuel for lighting and cooking in the UK and later in Germany. The product mixture has a specific enthalpy about half that of natural gas. The reaction **runs at 2000°C and 0.1 MPa** using an iron oxide catalyst. Coal is ground to 100μm particles and suspended in the O_2 and H_2O streams. The **heat of reaction at 25°C and 0.101 MPa is -91 kJ/mole** using the stoichiometry in the balanced reaction given below. Consider that the reactants are fed at **200°C and 0.2 MPa** and the products are released at **2000°C and 0.1 MPa**. **95% of the coal is converted to CO at this temperature.**

a) Is this reaction, under these conditions, exothermic or endothermic?
b) What Q is required per mole of the given stoichiometry?
   The heat capacities, C_p, are given in the table below. Ignore the temperature dependence of the heat capacity.
c) Calculate the heat needed per mole of O_2 to cool the exiting stream from 2000°C to 250°C. ***Consider all of the components for this step.***
   What could be done with this excess heat?
d) The raw gas exits the reactor after the heat exchanger at 250°C and 0.1 MPa. This gas stream must be compressed to 10 MPa for transmission by pipe to customers. For an adiabatic compressor with an efficiency, $\eta = 0.85$, what power in Watts (or J/s) will be needed if the gas output is 5 kg/s (enough to feed 700 houses)? ***Consider that the exit gas stream is just H_2 and CO in a 1:3 molar ratio for this step. Use the molar average C_p and molecular weight. The molecular weights are in the table below.***
   -First calculate the power for $\Delta S = 0$, then apply the efficiency to obtain the actual work.
e) What will be the exit temperature for the compressor?
f) This is not the normal process for a large compression process. Can you guess at how this last compression/cooling would normally be carried out? (Extra credit)

$$3C \text{ (i.e., coal)} + O_2 + H_2O \rightarrow H_2 + 3CO$$

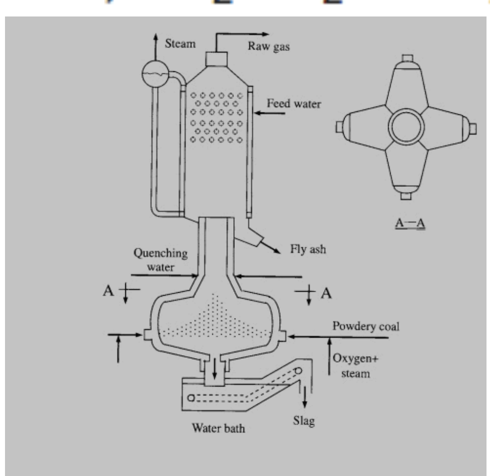

Figure 8.2. Koppers–Totzek powdery coal gasifier.

Moles	C (s)	O2 (g)	H2O (v)	H2 (g)	CO (g)	T, °C
in	3					
out						
Cp, J/(moleK)	21.2	29.3	33.6	29.2	29.2	-
Molecular Weight g/mole	12	32	18	2	28	-
Part a: Endo or Exo?						
Part b: Q =						
Part c: Q =						
Part c: What to do with this heat?						
Part d: Power in Watts?						
Part e: Exit Temperature =						
Part f: Alternative Compression Method (Extra Credit)						

1 atmosphere is 14.7 psi, 1.01 bar, 0.101 MPa, 760 mmHg, 29.9 inHg

Gas Constant, R

$= 8.31447$ J/mole-K $= 8.31447$ cm^3-MPa/mole-K $= 8.31447$ m^3-Pa/mole-K

$= 8{,}314.47$ cm^3-kPa/mole-K $= 83.1447$ cm^3-bar/mole-K $= 1.9859$ Btu/lbmole-R(see note 1)

$= 82.057$ cm^3-atm/mole-K $= 1.9872$ cal/mole-K(see note 2) $= 10.731$ ft^3-psia/lbmole-R

Process Type	Work Formula (ig)
Isothermal	$W_{EC} = -\int P dV = -RT\int \frac{dV}{V} = -RT\ln\frac{V_2}{V_1}$ (ig)
Isobaric	$W_{EC} = -\int P dV = -P(V_2 - V_1)$ (ig)
Adiabatic and reversible	$W_{EC} = -\int P dV = -\int \text{const}\frac{dV}{V^{(C_P/C_V)}}$ (*ig) or $\Delta U = C_V(T_2 - T_1) = W_{EC}$ (*ig) $\frac{T_2}{T_1} = \left(\frac{P_2}{P_1}\right)^{(R/C_P)} = \left(\frac{V_1}{V_2}\right)^{(R/C_V)}$ (*ig)

$Q_{rev} = \Delta U$ for isochoric (constant volume) 4.17

$dU = C_v\, dT$ for isochoric (constant volume)

$C_p = C_v + R$ (exact for ideal gas)

$\Delta H = \Delta U + \Delta(PV) = \Delta U + R(\Delta T)$ (exact for ideal gas)

$T_2/T_1 = (P_2/P_1)^{R/Cp} = (V_1/V_2)^{R/Cv}$

$$\boxed{d\underline{S} \equiv \frac{d\underline{Q}_{rev}}{T_{sys}}}$$

$$\boxed{\Delta S = \int_{T_1}^{T_2} \frac{C_P}{T} dT}$$

❶ Constant pressure.

$$\boxed{\Delta S = \int_{T_1}^{T_2} \frac{C_V}{T} dT}$$

❶ Constant volume.

$$\boxed{\Delta S^{ig} = R\ln\left[\frac{V_2}{V_1}\right]} \text{ or } \boxed{\Delta S^{ig} = -R\ln\left[\frac{P_2}{P_1}\right]}$$

❶ Isothermal.

$$\boxed{\Delta S = \int_{state\ 1}^{state\ 2} \frac{dQ_{rev}}{T_{sys}} = 0}$$ for reversible process only.

$$\boxed{\Delta S^{vap} = \frac{\Delta H^{vap}}{T^{sat}}} \text{ and } \boxed{\Delta S^{fus} = \frac{\Delta H^{fus}}{T_m}}$$

❶ Adiabatic *and* reversible.

$$\boxed{dS^{ig} = \frac{C_V}{T}dT + \frac{R}{V}dV}$$

$$\boxed{\Delta S^{ig} = C_V\ln\frac{T}{T^i} + R\ln\frac{V}{V^i}} \text{ or } \boxed{\Delta S^{ig} = C_P\ln\frac{T}{T^i} - R\ln\frac{P}{P^i}}$$

$$\boxed{\left(\frac{\partial S}{\partial T}\right)_V = \frac{C_V}{T}}$$

$$\boxed{\left(\frac{\partial S}{\partial T}\right)_P = \frac{C_P}{T}}$$

Moles	C (s)	O2 (g)	H2O (v)	H2 (g)	CO (g)	T, °C
in	3	1	1	0	0	200
out	0.15	0.05	0.05	0.95	2.85	2000
Cp, J/(moleK)	21.2	29.3	33.6	29.2	29.2	-
Molecular Weight g/mole	12	32	18	2	28	-

Part a: Endo or Exo?	Endo thermic
Part b: Q =	123 kJ per mole
Part c: Q =	205 kJ per mole
Part c: What to do with this heat?	Heat Reactants
Part d: Power in Watts?	11.5 MW
Part e: Exit Temperature =	1930 °C (2210 K)

Answer Quiz 4

a)

		moles	C_p J/mol K	$\Sigma n C_p$ J/K	ΔT K	$\Sigma n C_p \Delta T$ kJ
	C	0.15	21.2			
	O_2	0.05	29.3	117 J/K	1980 K	232 kJ
Products	H_2O	0.05	33.6			
	H_2	0.95	29.2			
	CO	2.85	29.2			
	C	3.00	21.2			
Reactants	O_2	1.00	29.3	126.5 J/K	175 K	−22.1 kJ
	H_2O	1.00	33.6			
	H_2	0	29.2			
	CO	0	29.2			
ΔH^o_{Rxn}		0.95		−91 kJ/mole		−86.5 kJ

$Q_{Rxn} = 123$ kJ

Per 1 mole O_2

Endothermic

b) $Q_{Rxn} = 123$ kJ

c) $(\Sigma n C_p)\Delta T = 117 \frac{J}{K}$ 1750 K = 205 kJ

This could be used to heat the reactants

d) C_p is the same for H_2 & CO

$C_p = 29.2$ J/mol K

$\langle M_w \rangle = \frac{(3 \cdot 28\,g/mole + 1 \cdot 2\,g/mol)}{4} = 21.5$ g/mole

$1000\frac{g}{kg}$ 5 kg/s / 21.5 g/mole = 233 $\frac{mole}{s}$

For $\Delta S = 0$

$$0 = C_p \ln\left(\frac{T_F}{T_1}\right) - R \ln\left(\frac{P_2}{P_1}\right)$$

$$T_F' = T_1 \left(\frac{P_2}{P_1}\right)^{R/C_p} = 523K \left(\frac{10\,MPa}{0.1\,MPa}\right)^{\frac{1}{3.5}} = 1950K$$
$(1680°C)$

$$\Delta H' = W_s' = 29.2 \frac{J}{mol\,K} (1680°C - 250°C)$$
$(Q=0)$

$$= 41.8\ kJ/mole$$

$$\Delta H = \frac{\Delta H'}{\eta} = \frac{41.8\ kJ/mole}{0.85} = 49.2\ kJ/mole$$

$$\text{Power} = 49.2\ kJ/mole \cdot 233\ mole/s = 11.5\ MW$$

e) $$\Delta H = C_p(T_f - T_i) = 49.2\ kJ/mole$$

$$T_f = \frac{49.2\ kJ/mole \cdot 1000\ J/kJ}{29.2\ J/mole\,K} + 250°C$$

$$= 1930°C$$
$(2210K)$