Note there will be no part marking below what has been shown.

1. A coal burning burner is fed with powdered coal (assume pure carbon) preheated to 1800K and dry air (N2:O2=79:21, by volume) preheated to 1200K. The coal to air ratio is such that the product is only a gas containing CO and N2. Perform a material balance and a heat balance and calculate the adiabatic flame temperature (of the product gas).
   Take only 1 mol (12g) carbon as the mass basis. You need to present data as **mass and heat balance tables**. (Only the entries in the table may be seen for valuation) **4 marks**

Solution:

Reaction: $C_{(s)} + \frac{1}{2}O_{2(g)} = CO_{(g)}$; $\Delta H_{298} = -111000\ J/mol$

$(12g) + 16(g) = 28(g)$

Input	mol	mass, g	output	mol	mass, g
C	1	12.	CO	1	28
Air: O_2	½	16	N_2	1.8810	52.67
N_2	$\frac{1}{2} \times \frac{0.79}{0.21} = 1.8810$	52.67			
		80.67			80.67

1 mark for correct & complete table

Input			Output		
Sensible Heat			Sensible Heat		
C 1800K	1(23.5×1800 − 11800)	30500	CO	1(36.6T − 16400)	72439
Air, 1200K O_2	½(36.2T − 13500)	14970	N_2	1.881(36.4T − 16500)	135157
N_2	1.881(36.4T − 16500)	51126			
Reaction Heat	−1(−111000)	111000	Loss	adiabatic	0
		207596			207596

1 mark for correct completed table
½ mark if R.H.S entries not made.

$T(36.6 + 68.47) - (16400 + 31037) = 207596$.

$T = \frac{207596 + 47437}{105.07} = 2427.3K = 2154.2°C$

(±5°) 2 marks

2. 1 mole of a super-cooled material is adiabatically contained at 400 K at constant pressure. If it spontaneously freezes, what is the final temperature? What fraction of the material freezes?

$\Delta H_m^o = 2000 \frac{J}{mol}. at\ T_m = 600K$
$C_p: liq: 34.7 - 9.2x10^{-3}T$ J/mol.K
$Sol: 18.5 + 2.6x10^{-3}$ T J/mol.K

[Note that starting from a temperature lower than the melting point, an adiabatically contained material cannot cross the melting point by releasing the latent heat and heating itself. This would violate the second law as we will see later. **Hence the maximum temperature can be 600K. It can be lower**]. **2marks**

+2 marks bonus, *if the numerical answer is rigorous conceptually ! There is a standard mistake that people commit.*

Solution:

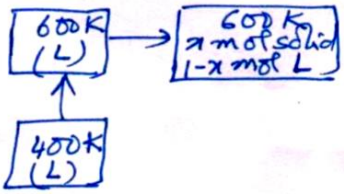
There are two options: (i) Latent heat released is sufficient to heat products to m.pt.: 600K; some liquid remains.

(ii) Even after full solidification; temp. does not reach 600K.

Explore option(i): Final temp 600K. Fraction solidified: x.

Adiabatic & constant pr; $q_p = \Delta H = 0$.

Since enthalpy calculation, path does not matter.

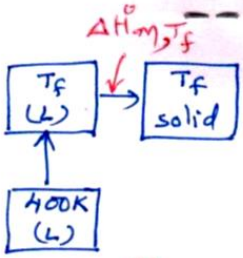


$$\Delta H = \int_{400}^{600} C_{p,L}\, dT + -(\Delta H^\circ_{m,600K}).x$$

$$= \left[34.7T - \frac{9.2\times10^{-3}}{2}T^2\right]_{400}^{600} - 2000x$$

$$= 6940 - 920 - 2000x = 0. \Rightarrow x = 3.01.$$ Not possible. Premise wrong

Option(ii) $x = 1$, T_f unknown.



$$34.7(T_f - 400) - \frac{9.2\times10^{-3}}{2}(T_f^2 - 400^2) = 2000$$

$$-4.6\times10^{-3}T_f^2 + 34.7T_f - (13800 - 736 + 2000) = 0$$

$$\boxed{T_f = 465.1 \text{ and } x = 1}$$ ① mark

[Award 2 marks, if option(ii) directly tried]

BONUS Question: (no part marking)

The error in the above is that $\Delta H^\circ_{m,465.1K} = \Delta H^\circ_{m,600K}$.

Calculate ΔH°_m at T_f : Kirchoff's Law.

$$S \to L;\ \Delta H^\circ_{m,T_f} - \Delta H^\circ_{m,600} = \int_{600}^{T_f}[C_{p(L)} - C_{p(S)}]\,dt$$

$$= \int_{600}^{T_f}(16.2 - 11.8\times10^{-3}T)\,dT$$

$$= 16.2(T_f - 600) - \frac{11.8\times10^{-3}}{2}(T_f^2 - 600^2)$$

Heat Balance therefore is:

$$34.7(T_f - 400) - 4.6\times10^{-3}(T_f^2 - 400^2) = 2000 + 16.2(T_f - 600) - \frac{11.8\times10^{-3}}{2}(T_f^2 - 600^2)$$

2 marks if this eqn. written correctly

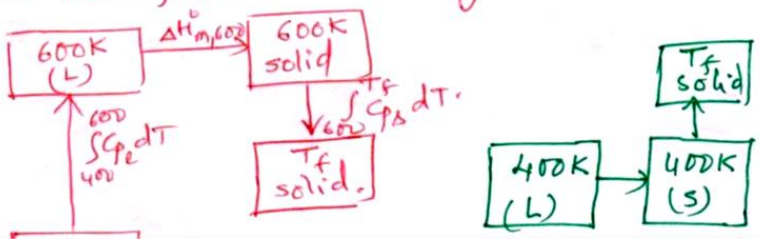
$$T_f^2\left(-4.6\times10^{-3} + \frac{11.8\times10^{-3}}{2}\right) + T_f(34.7 - 16.2) + (-13800 + 736 - 2000 + 9720 - 4248) = 0$$

$$7.2\times10^{-3}T_f^2 + 18.5T_f - 9592 = 0$$

$$T_f = \frac{-18.5 \pm 24.870}{2\times7.2\times10^{-3}} = 396.9$$

Significant difference? $\Delta H^\circ_{m,400K \text{ to } 442K} \approx -60$ J

Alternatively, one can follow the following scheme.



3. A mixture of steam at **400K** and oxygen at **300K**, both at 1 atm., react with a bed of graphite granules at **1000K** to yield a mixture of H_2 and CO at **1000K**. Calculate the composition of the CO/H_2 mixture, if the above process should be adiabatic (i.e. no heat effect). **Answer in tables** **4 marks**

Further data

	$H_T^o - H_{298}^o$, J/mol	ΔH_{298}^f, J/mol
CO	36.6T - 16400	-111000
CO_2	61.0T - 30500	-394000
$H_2O(g)$	47.4T - 22200	-242000
N_2	36.4T - 16500	-
O_2	36.2T - 13500	-
C	23.5T - 11800	-
H_2	35.2T - 17200	-

Note : $H_T^o - H_{298}^o = \int_{298}^{T} C_p \, dT$; **that is, it is an integrated expression.**

Basis: Take 1 k mol H_2O; x k mol O_2

Input	k mol	kg			
H_2O	1	18	CO	$1+2x = 2.589$	72.49
O_2	$x = 0.79433$	25.42	H_2	1	2
C	$1+2x = 2.589$	31.06			
		74.48			74.49

1 mark correct & complete

$H_2O + C = H_2 + CO$; $\Delta H^\circ_{298} = -111000 + 242000 = 131000$

		kJ			
H_2O (400K)	$1(47.4\times400 - 22200)$ (-3240)	-5240	CO	$(1+2x)(36.6\times1000 - 16400)$ (20200)	52291
O_2	$x(36.2\times300 - 13500)$ (-2640)	-2097	H_2	$1(35.2\times1000 - 17200)$ (18000)	18000
C	$(1+2x)(23.5\times1000 - 11800)$ (11700)	30287			
Rkn Ht 298K	$-131000 + (1+2x)\times 111000$	45341		$x = 0.7943$ ±0.01: 2 marks	
		70291			70291

1 mark correct & complete

$x(-2640 + 23400 + 222000 - 40400) = 20200 + 18000 + 3240 - 11700 + 131000$

NOTE : H2O +C = H2+CO ; $\Delta H_{298} = H^f_{CO} - H^f_{H2O}$ (since at 298K, $H_{element} = 0$)