1. Five moles of a monatomic ideal gas are contained adiabatically at 50 atm pressure and 300 K. The pressure is suddenly released to 10 atm, and the gas undergoes an irreversible expansion during which it performs 4000 joules of work. Show that the final temperature of the gas after the irreversible expansion is greater than that which the gas would attain if the expansion from 50 to 10 atm had been conducted reversibly. Calculate the entropy produced as a result of the irreversible expansion.

Answer

Given:

State 1: P_1 = 50 atm, T_1 =300K, n= 5 moles

Lets take reversible process takes the gas from state 1 to state 2 and

Irreversible process takes the gas from state 1 to state 3

State 2: n= 5 moles, P_2 =10 atm

State 3: n= 5 moles, P3 =10 atm

In the initial state 1, V_1= nRT_1/P_1 = (5 x 0.08206 x 300)/50 = 2.46 lit

If the adiabatic expansion from 50 to 10 atm is carried out reversibly, then the process path follows PV^{γ} =constant, and in the final state 2,

V_2 = $((50 \times 2.46^{5/3})/10)^{3/5}$ =6.47 litres

T2 =(10 x 6.47)/(5 x 0.08206) = 158K

For the irreversible process, which takes the gas from the state 1 to the state 3, as $q=0$,

ΔU = $-W$=-4000 =$-nC_v(T_3-T_1)$

and hence T_3=236 K, which is higher than T_2.

As the irreversible expansion from state 1 to state 3 was conducted adiabatically, no heat entered the system, and hence the difference between the entropy at state 3 and the entropy at state 1 is the entropy created, S_{irr} as a result of the irreversible process.

As the reversible adiabatic expansion from state 1 to state 2 is isentropic,

$S_3-S_1 = S_3-S_2$

For the reversible isobaric expansion from state 2 to state 3

$dS = nC_p dT/T$

Change in entropy from state 1 to state 3 =

$= 5 \times 2.5 \times 8.3144 \times \ln(236/158) = 42$ J/K

2. Calculate the adiabatic flame temperature of a gas having 20% CO and 80% N_2 when burnt with 150% excess air. Both the reactants are at 25°C. The adiabatic flame temperature is that temperature reached if all of the heat of the oxidation reaction is used to increase the temperature of the products of the reaction. Air is 21 molar percent O_2 and 79 molar percent N_2.

Data:

$\Delta H°_f$ of CO_2 = -94052 cal/gmol
$\Delta H°_f$ of CO = -26412 cal/gmol
Mean heat capacities in cal/gmol.°C are CO_2 = 12, O_2 = 7.9, N_2 = 7.55

Answer
1 mole of gas (having 20% CO and 80% N_2)
Combustion reaction:
CO + 1/2 O_2 ⟶ CO_2
Heat of reaction at 25°C for the above reaction is calculated as:
Heat of reaction = heat of formation of products - heat of formation of reactants
= -94052 - (-26412) = -94052 + 26412 = -67640 cal/gmol of CO converted
This represents exothermic heat of reaction.
Total heat liberated = 67640 x 0.2 = 13528 cal.
If a base temperature of 25°C is assumed, enthalpy of reactants at 25°C = 0 cal
Total enthalpy of product stream = enthalpy of reactants + heat added by

reaction = 0 + 13528 = 13528 cal.
This enthalpy rise of product stream with respect to feed is accomplished by a temperature increase, if the reaction is in adiabatic conditions.
Constituents of product stream are estimated as follows:
CO_2 in the product stream = 0.2 gmol
O_2 theoretically needed = 0.2 x 0.5 = 0.1 gmol.
O_2 actually entering (150% excess) = 0.1 x 2.5 = 0.25 gmol
N_2 entering along with O_2 in the air = 0.25 x 79/21 = 0.9405 gmol
O_2 in the leaving gases (assuming complete combustion of CO to CO_2) =
  0.25 - 0.1 = 0.15 gmol
N_2 in the leaving gases = 0.9405 + 0.8 = 1.7405 gmol.
Adiabatic temperature (T) is calculated as follows:
13528 = 0.2 x 12 x (T - 25) + 0.15 x 7.9 x (T - 25) + 1.7405 x 7.55 x (T - 25)
i.e., 13528 = 16.726 (T - 25)
808.8 = T - 25
T = 808.8 + 25 = 833.8°C
Adiabatic flame temperature = 833.8°C

3. The analysis of 15000 litre of gas mixture at standard conditions is as follows:
CO_2 = 9.5% ; SO_2 = 0.5% ; O_2 = 12.0% ; N_2 = 78.0%.
How much heat must be added to this gas to change its temperature from 25°C to 700°C?
Data: Specific heat values in kcal/(kmol.°K)

Gas	CO_2	SO_2	O_2	N_2
C_p at 25°C	8.884	9.54	7.017	6.961
C_p at 700°C	11.303	11.66	7.706	7.298

Answer
15000 litre of gas
22.4 litre is occupied by 1 gmol of gas at at 0°C.
therefore, number of gmol of gas in the volume of 15000 litre at 25°C, is estimated as:
PV = nRT (Ideal gas equation)
From the above equation,
$n_2 P_1 V_1 / T_1 = n_1 P_2 V_2 / T_2$
here P_1 and P_2 are the same.
Therefore,
n_2 x 22.4 / 273 = 1 x 15000 / (273 + 25)
n_2 = 613.5 gmol = 0.6135 kmol

Component	Mole fraction	No of moles, kmol
CO_2	0.095	0.6135 x 0.095 = 0.0583
SO_2	0.005	0.6135 x 0.005 = 0.0031

O_2	0.12	0.6135 x 0.12 = 0.0736
N_2	0.78	0.6135 x 0.78 = 0.4785

Heat required (H) to raise the temperature from 25°C to 700°C is given by,
$H = n_i C_{Pmi}(T_2 - T_1) = n_i C_{Pmi} (700 - 25)$
Where n_i is the moles of component 'i', and C_{Pmi} is the mean molal specific heat of component 'i'.
The calculations are shown in the following table.

Component	kmol	C_P at 25°C kcal/(kmol.°K)	C_P at 700°C kcal/(kmol.°K)	C_{Pm} kcal/(kmol.°K)	Heat to be added, kcal
CO_2	0.0583	8.884	11.303	(8.884 + 11.303)/2 = 10.0935	0.0583 x 10.0935 x (700 - 25) = 397.2
SO_2	0.0031	9.54	11.66	10.6	22.18
O_2	0.0736	7.017	7.706	7.3615	365.72
N_2	0.4785	6.961	7.298	7.1295	2302.74
				Total heat to be added	**3087.84 kcal**