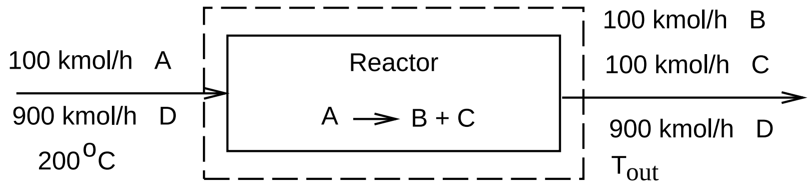
Chemical Engineering 1h

Mass and Energy Balances

Model Solutions to Tutorial 2

1. a)



	A	→	B	+	C
moles	1		1		1
kmol/h	100		100		100

The extent of reaction, ξ, is 100kmol/h and the heat of reaction, Δh_R°, is –36kJ/mol or –36000kJ/kmol.

We can first check to see whether the average heat capacity of the products is equal to that of the reactants. If so, we can use the simplified enthalpy balance relationship.

$$\sum_i \nu_i.c_{p,i} = (-1 \times 40) + (1 \times 20) + (1 \times 20) = 0$$

If the reactor is **isothermal**, $T_{in} = T_{out} = 200°C$

$$Q = \xi.\Delta h_R^{\circ} = \frac{100\text{kmol/h}}{3600\text{s/h}} \times (-36,000)\text{kJ/kmol} = -1000kW = -1MW$$

The fact that Q is negative indicates that heat is removed. The rate of heat removal is 1MW.

b) Under **adiabatic** conditions, no heat is removed or work done. Therefore all of the heat of reaction leaves the reactor with the products.
Here

$$\sum_i f_i.c_{p,i}.(T_{out} - T_{in}) + \xi.\Delta h_R^{\circ} = 0$$

$$\{\frac{1000}{3600} \times 40 \times (T_{out} - 200)\} + \{\frac{100}{3600} \times (-36000)\} = 0$$

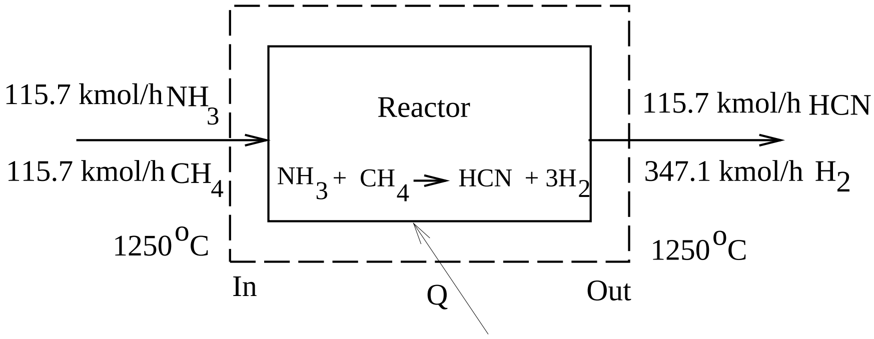
$$T_{out} = \frac{1000}{(\frac{100}{9})} + 200 = 290°C$$

If the reactant were introduced as a pure stream into the reactor, all of the thermal energy would leave the reactor in B & C. These would leave the reactor at a temperature of 1100°C (i.e. the temperature rise would be ten times as large). The inert substance D helps to moderate the temperature rise by absorbing a substantial amount of heat.

$$\{\frac{100}{3600} \times 40 \times (T_{out} - 200)\} + \{\frac{100}{3600} \times (-36000)\} = 0$$

$$T_{out} = \frac{1000}{(\frac{10}{9})} + 200 = 1100°C$$

2.



	CH_4	+	NH_3	$\rightarrow$	HCN	+	3 H_2
moles	1		1		1		3
kmol/h	115.7		115.7		115.7		347.1

Assuming an 8000hour working year, the extent of reaction, ξ, is $\frac{25000}{8000\times 27} = 115.7$kmol/h. The heat of reaction, Δh_r°, is 251.2 MJ/kmol.

We can first check to see whether the average heat capacity of the products is equal to that of the reactants. If so, we can use the simplified equations as presented in the lecture.

$$\sum_i \nu_i . c_{p,i} = (-1 \times 75) + (-1 \times 60) + (1 \times 45) + (3 \times 30) = 0$$

If the reactor is **isothermal**, $T_{in} = T_{out} = 1250°C$

$$Q = \xi . \Delta h_R^{\circ} = \frac{115.7\text{kmol/h}}{3600\text{s/h}} \times (251.2\text{MJ/kmol}) = 8.08MW$$

The heat duty is therefore 8.08MW. The rate of heat removal is

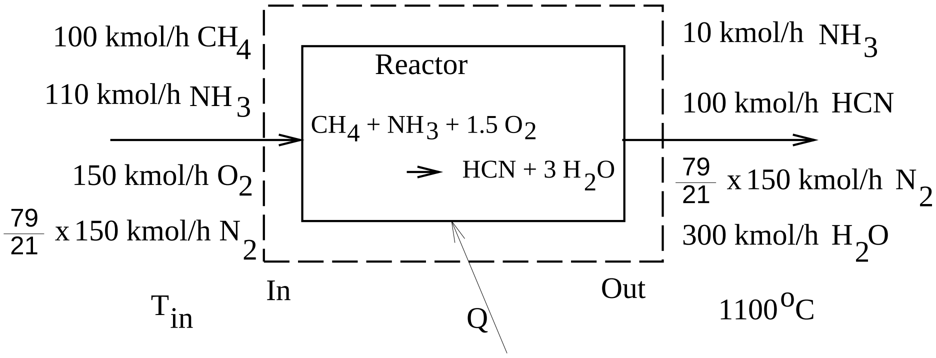
$$Q = U.A.\theta_{LM}$$

where the overall heat transfer coefficient, U = 300Wm^{-2}K^{-1} and the log mean temperature difference $\theta_{LM} = 150°C$ (θ is constant at 150°C throughout the reactor/heat exchanger.).

$$A = \frac{Q}{U.\theta_{LM}} = \frac{8.08 \times 10^6}{300 \times 150} = 180m^2$$

In order to choose the number and diameter of tubes, we need to ensure that the flow in the tubes will be turbulent. With ceramic tubes, especially ones to be internally coated with catalyst, there is likely to be a minimum size somewhere around 40mm diameter. Other factors to be considered are the pressure drop in the tubes and the ability to support long tubes.

3.



Assuming a basis of 100 kmol/h CH_4 feed to the reactor

	CH_4	+	NH_3	+	1.5 O_2	→	HCN	+	3 H_2O
moles	1		1		1.5		1		3
kmol/h	100		100		150		100		300

The extent of reaction, ξ, is 100kmol/h. The heat of reaction, $\Delta h_r^{\ominus}$, is –606.2 MJ/kmol.

We can first check to see whether the average heat capacity of the products is equal to that of the reactants. If so, we can use the simplified equations as presented in the lecture.

$$\sum_i \nu_i.c_{p,i} = (-1 \times 75) + (-1 \times 60) + (-1.5 \times 30) + (1 \times 45) + (3 \times 45) = 0$$

All of the CH_4 and O_2 reacts and NH_3 is provided in 10% excess. The feed to the reactor therefore contains 100kmol/h CH_4, 110kmol/h NH_3, 150kmol/h O_2 and $\frac{79}{21} \times 150 =$ 564.3kmol/h N_2.

The reactor gauze is to be maintained at 1100°C. This is the same temperature as that at which the products leave the reaction zone. In addition, we are told that 50% of the heat of reaction is radiated from the gauze. Therefore

$$\sum_i f_i.c_{p,i}.(T_{out} - T_{in}) + \xi.\Delta h_R^{\ominus} = Q$$

where

$$Q = 0.5 \times \xi.\Delta h_R^{\ominus}$$

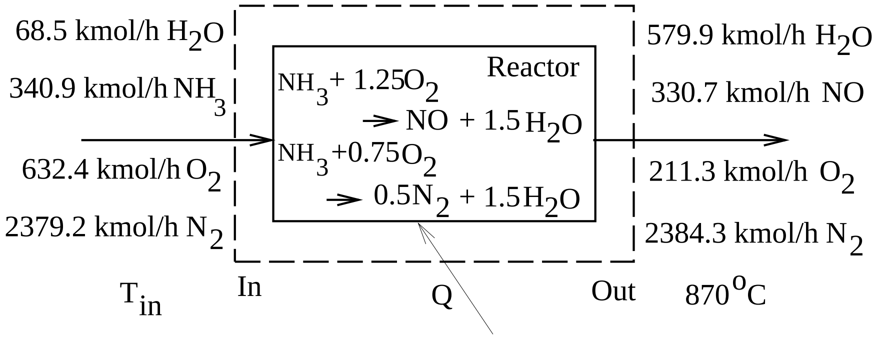
Thus

$$\{(\frac{100}{3600} \times 75) + (\frac{110}{3600} \times 60) + (\frac{150}{3600} \times 30) + (\frac{564.3}{3600} \times 30)\}.(1100 - T_{in})$$
$$+\frac{100}{3600} \times (-606200) = 0.5 \times \frac{100}{3600} \times (-606200)$$

or

$$(2.083 + 1.833 + 1.25 + 4.703).(1100 - T_{in}) - 16840 = -8420$$
$$9.87 \times (1100 - T_{in}) = 8420$$
$$T_{in} = 1100 - \frac{8420}{9.87} = 247°C$$

4.



Mass Balance

The reactant stream contains 340.9kmol/h NH_3, 2379.2kmol/h N_2, 632.4kmol/h O_2 and 68.5kmol/h H_2O.

97% of the ammonia reacts to give NO:

	NH_3	+	$1.25\ O_2$	$\rightarrow$	NO	+	$1.5\ H_2O$	(1)
moles	1		1.25		1		1.5	
kmol/h	330.7		413.4		330.7		496.1	

and 3% reacts to give N_2:

	NH_3	+	$0.75\ O_2$	$\rightarrow$	$0.5\ N_2$	+	$1.5\ H_2O$	(2)
moles	1		0.75		0.5		1.5	
kmol/h	10.2		7.7		5.1		15.3	

The product stream contains 2384.3kmol/h N_2, 211.3kmol/h O_2, 579.9kmol/h H_2O and 330.7kmol/h NO.

For reaction 1, the extent ξ_1 = 330.7kmol/h and heat of reaction $\Delta h^{\ominus}_{R,1}$ = -227MJ/kmol.
For reaction 2, the extent ξ_2 = 10.2kmol/h and heat of reaction $\Delta h^{\ominus}_{R,2}$ = -409MJ/kmol.

Enthalpy Balance

The enthalpy balance equation for an adiabatic reactor, assuming that the average specific heat of the products is similar to that of the reactants, is

$$\sum_i f_i.c_{p,i}.(T_{out} - T_{in}) + \sum_k \xi_k.\Delta h^{\ominus}_{R,k} = 0$$

The temperature of the gauze and hence of the products is 870°C.

$$\{(\frac{340.9}{3600} \times 60) + (\frac{2379.2}{3600} \times 30) + (\frac{632.4}{3600} \times 30) + (\frac{68.5}{3600} \times 45)\}.(870 - T_{in})$$
$$+\{(\frac{330.7}{3600} \times -227000) + (\frac{10.2}{3600} \times -409000)\} = 0$$

$$(5.682 + 19.827 + 5.27 + 0.856).(870 - T_{in}) + (-20852 - 1159) = 0$$

$$31.635 \times (870 - T_{in}) - 22011 = 0$$

$$T_{in} = 870 - \frac{22011}{31.635} = 174°C$$