General Economic Factors to Consider

The rate of reaction and percentage yield must be high enough to give a sufficient daily yield of product.

Having a fast rate of reaction does not mean necessarily that a good yield will be achieved. Sometimes a compromise is needed.

Optimum conditions of temperature and pressure are used that give the **lowest cost**, rather than the fastest reaction or highest percentage yield.

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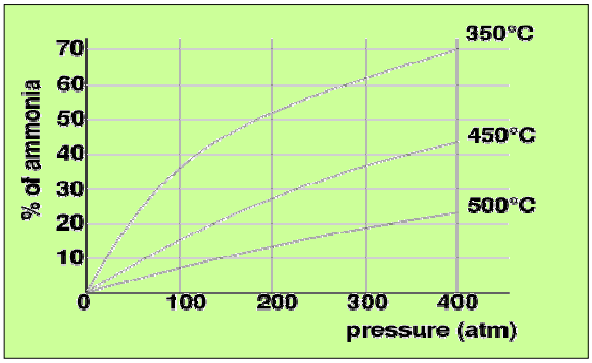
Haber Process: Effect of Temperature

$N_2 + 3H_2 \rightleftharpoons 2NH_3$ ΔH = -ve exo



High temperatures give a low yield of ammonia

If temperature is increased the **equilibrium will shift to the left to oppose** this and move in the **endothermic** direction to try and reduce the temperature by absorbing heat.

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Effect of Temperature

For this reaction a **low temperature will give a high yield** of ammonia.

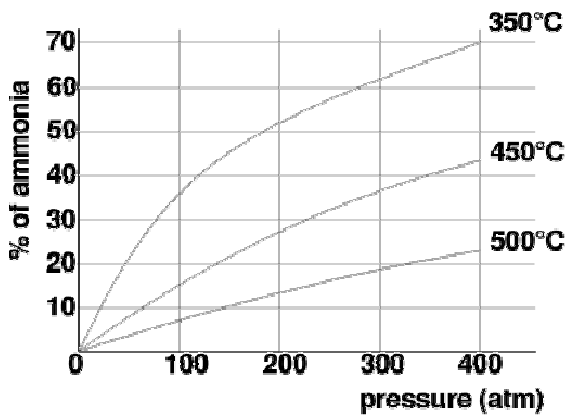
However, **low temperatures will mean the rate of reaction is slow.** So we need to use a compromise temperature that gives both a reasonable yield and rate

- A temperature in the region of 450°C is used
- 450 °C is an optimum temperature that gives a fast reaction without giving a very small percentage yield

The higher the temperature, the higher the cost of the energy bill for electricity or fuel.

Haber Process: Effect of Pressure

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$



If pressure is increased then the equilibrium will move to reduce the pressure.

It will move to the side with the fewer molecules of gas. In this case towards the products

High Pressure gives a good yield of ammonia

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Effect of pressure

- A high pressure will give a good yield.
- Higher pressure increases the rate of reaction

•However, the higher the pressure used, the **higher the cost of the equipment needed to withstand the pressure**.

•The higher the pressure the **higher the electrical energy costs for pumps** to produce the pressure.

A moderately high pressure of between 200 – 1000 atmospheres is used.

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Other Factors

Iron Catalyst

Increases the rate of reaction BUT does not change yield.

reduces cost because the rate is increased so the reaction takes less time and lower temperatures can be used

Unreacted N_2 AND H_2 recycled back into the reactor

Reduces waste and lowers costs.

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Contact Process

Sulphuric acid is produced by the contact process

Stage 1: Sulphur is burnt in air

$S(s) + O_2(g) \rightarrow SO_2(g)$ $\Delta H = -297\ kJ\ mol^{-1}$

Stage 2: Sulphur dioxide is reacted with oxygen

$SO_2(g) + \frac{1}{2} O_2(g) \rightleftharpoons SO_3(g)$ $\Delta H = -98\ kJ\ mol^{-1}$

What effect would increasing temperature and pressure have on the yield of SO_3 and the rate of reaction?

A V_2O_5 catalyst is used. What effect it have on the yield of SO_3 and the rate of reaction?

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Contact Process (continued)

Why is the concentration of SO_2 kept high?

The conditions used are 450°C (moderately high) and 10 atm

Why is this temperature used?

Why is a much higher pressure not used?

Stage 3: Sulphur trioxide is dissolved in conc sulphuric acid

$SO_3(g) + H_2SO_4(l) \rightleftharpoons H_2S_2O_7(l)$ $\Delta H = -230\ kJ\ mol^{-1}$

$H_2S_2O_7(l) + H_2O(l) \rightarrow H_2SO_4(l)$

Stage 3 constantly removes the SO_3 formed in stage 2. What effect does this have the position of equilibrium in stage 2?

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Hydration of ethene

$CH_2{=}CH_{2\,(g)} + H_2O_{\,(g)} \rightleftharpoons CH_3CH_2OH_{(l)}$ $\Delta H = -45\ kJ\ mol^{-1}$

Essential Conditions

high temperature 300 °C (moderate temp)

high pressure 70 atm (moderate pressure)

strong acidic catalyst of concentrated H_3PO_4

Why are these conditions chosen?

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Hydration of ethene

- Low temp leads to high yield but slow rate
- High pressure leads to high yield and high rate but is expensive to produce high pressure (high electrical costs for pumping) and contain (expensive equipment to contain high pressure)
- Compromise temps and pressures used.
- High pressure also leads to unwanted polymerisation of ethene to polyethene
- At chosen conditions only 5% conversion, but a recycle is used to recycle the unreacted ethene.
- Conc Phosphoric acid catalyst speeds up rate of reaction

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Production of methanol from CO

$CO_{(g)} + 2H_{2(g)} \rightleftharpoons CH_3OH_{(g)}$ $\Delta H = -91\ kJ\ mol^{-1}$

What would be the likely industrial conditions for this reaction to give the best economics?

The CO used in this has traditionally been made from methane

$CH_{4\ (g)} + H_2O_{(g)} \rightleftharpoons CO_{(g)} + 3H_{2\ (g)}$ $\Delta H = +206\ kJ\ mol^{-1}$

What would be the likely industrial conditions for this reaction to give the best economics?

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Methanol carbon neutral fuel?

$CO_{(g)} + 2H_{2(g)} \rightleftharpoons CH_3OH_{(g)}$

The term carbon neutral refers to “an activity that has no net annual carbon (greenhouse gas) emissions to the atmosphere”

Why could methanol produced by the above reaction be classed as carbon neutral?

Would it be carbon neutral if the CO was produced from methane?

If the CO was formed from capturing CO_2 from the atmosphere, what conditions would be necessary for it to be truly carbon neutral?

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