Chem Factsheet

www.curriculum-press.co.uk Number 222

Compromise Conditions

INTRODUCTION

When a chemical substance is manufactured on a large scale, chemical theory can be used to predict the best experimental conditions (temperature, pressure, concentration etc) to **maximise** (a) the **yield** of the substance and (b) the **rate** of production of the substance.

However, in practice, the conditions predicted are not necessarily those used because they can often be contradictory for yield and rate optimizations.

Energy costs (for heating and pumping), equipment costs (to withstand high temperatures and pressures), labour costs, safety costs, environmental costs (e.g. carbon dioxide emissions during energy production and transport processes) and transport costs are also important because profit can only be maximised if such **costs are minimised.** Also, the best conditions for lowest costs might also be contradictory to those required to maximise yield and / or rate.

Labour costs are generally minimised by automating processes and using continuous processes rather than batch processes.

Transport costs are generally minimised by using local raw materials and distributing products in bulk.

As a result of combining all such considerations, it is usually necessary to adopt what are called "compromise conditions" of temperature and pressure. In general, these are adopted to produce an acceptable yield at an acceptable rate with acceptable costs, so that the overall process gives an acceptable profit.

Q1 FOR AN **ENDOTHERMIC** REACTION WHICH INVOLVES AN **INCREASE IN THE NUMBER OF GAS MOLECULES** FROM LEFT TO RIGHT
e.g. $CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$; $\Delta H = +178$ kJ mole^{-1}

Le Chatelier's Principle shows that a *higher yield of product* is favoured by a **LOWER / HIGHER** temperature and LOWER / **HIGHER** pressure.
However, using such *temperatures* would **DECREASE / INCREASE** energy, equipment, safety and environmental costs even though the rate of reaction would be **LOWER / HIGHER**.
Also using such *pressures* would **DECREASE / INCREASE** energy, equipment, safety and environmental costs but the rate of reaction would be **LOWER / HIGHER**.

Q2 FOR AN **ENDOTHERMIC** REACTION WHICH INVOLVES AN **DECREASE IN THE NUMBER OF GAS MOLECULES** FROM LEFT TO RIGHT
e.g. $6CO_2(g) + 7H_2O(g) \rightleftharpoons C_6H_{14}(1) + 9.5O_2(g)$; $\Delta H = +2162$ kJ mole^{-1}
Note : No such "real" reaction occurs so the idea of "compromise conditions" is purely academic here [1].

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Q3 FOR AN **EXOTHERMIC** REACTION WHICH INVOLVES AN **INCREASE IN THE NUMBER OF GAS MOLECULES** FROM LEFT TO RIGHT
e.g. $2H_2O_2(1) \rightleftharpoons 2H_2O(1) + O_2(g)$; $\Delta H = -98.8$ kJ mole^{-1}

Le Chatelier's Principle shows that a *higher yield of product* is favoured by a **LOWER / HIGHER** temperature and **LOWER / HIGHER** pressure.
Using such *temperatures* would **DECREASE / INCREASE** energy, equipment, safety and environmental costs but the rate of reaction would be **LOWER / HIGHER**.
Also using such *pressures* would **DECREASE / INCREASE** energy, equipment, safety and environmental costs but the rate of reaction would be **LOWER / HIGHER.**
The use of a catalyst is desirable in this case because it will allow the rate of reaction to be *higher* at a **HIGHER / LOWER** temperature and a **HIGHER / LOWER** pressure.

Q4 FOR AN **EXOTHERMIC** REACTION WHICH INVOLVES AN **DECREASE IN THE NUMBER OF GAS MOLECULES** FROM LEFT TO RIGHT
e.g. $N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$; $\Delta H = -92.2$ kJ mole^{-1}

Le Chatelier's Principle shows that a *higher yield of product* is favoured by a **LOWER / HIGHER** temperature and **LOWER / HIGHER** pressure.
Using such *temperatures* would **DECREASE / INCREASE** energy, equipment, safety and environmental costs but the rate of reaction would be **LOWER / HIGHER**.
Also using such *pressures* would **DECREASE / INCREASE** energy, equipment, safety and environmental costs even though the rate of reaction would be **LOWER / HIGHER**.
The use of a catalyst is desirable in this case because it will allow the rate of reaction to be *higher* at a **HIGHER / LOWER** temperature and a **HIGHER / LOWER** pressure.

EXAMPLE 1

Haber Process for making Ammonia

Ammonia is an important material for making nitric acid and is used to manufacture fertilisers.

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \; ; \; \Delta H = -92.2 \text{ kJ mole}^{-1}$$

Carried out at 300-550°C and 15-25 MPa using an Fe catalyst.

Q5 (a) Temperatures *below* 300°C are not used because, even though yield will be **LOWER / HIGHER** and energy, equipment, safety and environmental costs will be **LOWER / HIGHER**, the rate of reaction would be too **LOW / HIGH**.

(b) Temperatures *above* 300°C are not used because, even though rate will be **LOWER / HIGHER**, energy, equipment, safety and environmental costs will be **LOWER / HIGHER** and the yield would be too **LOW / HIGH**.

(c) Pressures *below* 15MPa are not used because, even though energy, equipment, safety and environmental costs will be **LOWER / HIGHER**, the yield and the rate of reaction would be too **LOW / HIGH**.

(d) Pressures *above* 25MPA are not used because, even though yield and rate will be **LOWER / HIGHER**, energy, equipment, safety and environmental costs will be too **LOW / HIGH**.

(e) The iron catalyst is used to allow an acceptable **YIELD / RATE** at a lower temperature.

EXAMPLE 2

Catalytic Cracking

Catalytic cracking of long-chain alkanes to produce smaller alkanes, cycloalkanes, alkenes and hydrogen is a very important process. The production of branched C8 hydrocarbons is particularly important in making petrol while alkenes are essential for making addition polymers.

$$\text{e.g. } C_{12}H_{26}(g) \rightleftharpoons C_8H_{18}(g) + 2C_2H_4(g) \; ; \; \Delta H = +225 \text{ kJ mole}^{-1}$$

Carried out at 500-600°C and 1.5-2.0 kPa using a Zeolite catalyst.

Q6 (a) Temperatures *below* 500°C are not used because, even though energy, equipment, safety and environmental costs will be **LOWER / HIGHER**, the yield and rate of reaction would be too **LOW / HIGH**.

(b) Temperatures *above* 600°C are not used because, even though rate and yield will be **LOWER / HIGHER**, energy, equipment, safety and environmental costs will be too **LOW / HIGH**.

(c) Pressures *below* 1.5kPa are not used because, even though energy, equipment, safety and environmental costs and yield will be **LOWER / HIGHER**, the rate of reaction would be too **LOW / HIGH**.

(d) Pressures *above* 2.0kPA are not used because, even though rate will be **LOWER / HIGHER**, energy, equipment, safety and environmental costs and yield will be too **LOW / HIGH**.

(e) The Zeolite catalyst is used to allow an acceptable **YIELD / RATE** at a lower temperature.

FURTHER QUESTION

Q7 Methanol is a useful liquid fuel that can be produced by direct combination of carbon monoxide and hydrogen.

$$CO(g) + 2H_2(g) \rightleftharpoons CH_3OH(g) \; ; \; \Delta H = -91 \text{ kJ mole}^{-1}$$

(a) Use Le Chatelier's Principle to explain why a low temperature and a high pressure favour a high yield of methanol in this reaction.

Low Temperature ______________________________

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High Pressure ______________________________

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(b) The industrial manufacture of methanol using this reaction is carried out at a temperature of 400°C under a pressure of 20 MPa in the presence of a Cr_2O_3/ZnO catalyst. Compare these conditions with your answer to part (a) and comment on why these conditions are used.

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ANSWERS TO QUESTIONS

Q1 HIGHER temperature and LOWER pressure. – would INCREASE energy, equipment – rate of reaction would be HIGHER. – would DECREASE energy, equipment – would be LOWER.

Q2 HIGHER temperature and HIGHER pressure. – would INCREASE energy, equipment – rate of reaction HIGHER. – would INCREASE energy, equipment, – would be HIGHER.

Q3 LOWER temperature and LOWER pressure. – would DECREASE energy, equipment, – rate of reaction LOWER. – would DECREASE energy, equipment – rate of reaction would be LOWER. – *higher* at a LOWER temperature and LOWER pressure.

Q4 LOWER temperature and HIGHER pressure. – would DECREASE energy, equipment, – rate of reaction LOWER. – would INCREASE energy, equipment – rate of reaction would be HIGHER. – *higher* at a LOWER temperature and LOWER pressure.

Q5 (a) – yield will be HIGHER – costs will be LOWER, – rate of – too LOW.
(b) – rate will be HIGHER, – costs will be HIGHER – yield too LOW.
(c) – costs will be LOWER, yield and rate – too LOW.
(d) – yield and rate HIGHER, – costs will be too HIGH.
(e) – acceptable RATE at a lower temperature.

Q6 (a) – costs will be LOWER, – yield and rate – too LOW.
(b) – rate and yield HIGHER – costs will be too HIGH.
(c) – costs will be LOWER, – yield and rate – too LOW.
(d) – yield and rate HIGHER, – costs will be too HIGH.
(e) – acceptable RATE at a lower temperature.

Q7 (a) Lowering the temperature causes the equilibrium to shift in the direction which releases heat energy and so counteracts the decrease in temperature. Hence it shifts in the exothermic direction. This means a shift towards the products and so increases the yield.

Raising the pressure causes the equilibrium to shift in the direction which lowers the total pressure and so counteracts the increase in pressure. Hence it shifts in the direction which involves a decrease in the number of gaseous molecules ($3 \rightarrow 1$). This means a shift towards the products and so increases the yield.

(b) The working temperature is high rather than low but the pressure is high, as predicted.

The higher temperature is used to give a higher rate of reaction even though this reduces the yield and increases energy costs. However, use of an even higher temperature would make the costs of reduced yield and energy economically unacceptable. The use of the catalyst minimises these adverse effects by achieving the acceptable rate of reaction without an excessive increase in temperature. Conversely, use of a lower temperature would decrease the rate of reaction unacceptably even though the yield would be increased and energy costs reduced. 400°C is the best compromise temperature.

The use of a high pressure increases yield and rate but also increases energy costs for pressurisation and equipment costs. However, use of an even higher pressure to increase yield and rate even more would make these costs economically unacceptable. The pressure adopted is high enough to give an economically acceptable yield and rate. Conversely, use of a lower pressure would decrease the yield and rate of reaction unacceptably even though the energy and equipment costs would be reduced. 20MPa is the best compromise pressure.

Acknowledgements: *This Factsheet was researched and written by Mike Hughes.*
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