Chapter 5: macroscopic aspects

1. Ammonia synthesis

**DOCUMENT 1: The Haber-Bosch process**

The Haber process, also called the Haber–Bosch process, is an artificial nitrogen fixation process and is the main industrial procedure for the production of ammonia today. It is named after its inventors, the German chemists Fritz Haber and Carl Bosch, who developed it in the first half of the 20th century. The process converts atmospheric nitrogen (N2) to ammonia (NH3) by a reaction with hydrogen (H2) using a metal catalyst under high temperatures and pressures:

$$N\_{2(g)}+3H\_{2\left(g\right)}⇌2NH\_{3(g)}$$

This conversion is typically conducted at 15–25 MPa (150–250 atm) and between 400–500 °C, as the gases (nitrogen and hydrogen) are passed over four beds of catalyst, with cooling between each pass so as to maintain a reasonable equilibrium constant. On each pass only about 15% conversion occurs, but any unreacted gases are recycled, and eventually an overall conversion of 97% is achieved.

Pressure is the obvious choice to favor the forward reaction because there are 4 moles of reactant for every 2 moles of product, and the pressure used (15–25 MPa, 150–250 bar) alters the equilibrium concentrations to give a profitable yield.

Economically, pressure is an expensive commodity. Pipes, valves, and reaction vessels need to be strengthened, and there are safety considerations of working at 20 MPa. In addition, running pumps and compressors takes considerable energy. Thus, the compromise used gives a single pass yield of around 15%.

Another way to increase the yield of the reaction would be to remove the product (i.e. ammonia gas) from the system. In practice, gaseous ammonia is not removed from the reactor itself, since the temperature is too high; it is removed from the equilibrium mixture of gases leaving the reaction vessel. The hot gases are cooled enough, whilst maintaining a high pressure, for the ammonia to condense and be removed as liquid. Unreacted hydrogen and nitrogen gases are then returned to the reaction vessel to undergo further reaction.

**Source: https://en.wikipedia.org/wiki/Haber\_process**

**DOCUMENT 2: Equilibrium constants under 200 bar**

|  |  |
| --- | --- |
| **Temperature (°C)** | **K°(T)** |
| 300 | $$4.34 × 10^{-3}$$ |
| 400 | $$1.64 × 10^{-4}$$ |
| 450 | $$4.51 × 10^{-5}$$ |
| 500 | $$1.45 × 10^{-5}$$ |
| 550 | $$5.38 × 10^{-6}$$ |
| 600 | $$2.25 × 10^{-6}$$ |

### Problem solving:

Using the documents, identify all parameters that enable to increase the yield of the ammonia synthesis reaction?

Activity summary

What you must remember:

- yield

- pressure, temperature

- reactant, product

Skills linked to the curriculum:

|  |  |
| --- | --- |
| **Compétences** | **Capacités à maitriser** |
| * APP
 | Lire des documents scientifiques |
| * ANA
 | Déterminer le rendement d’une synthèse en une ou plusieurs étapes. Identifier les facteurs permettant d’optimiser le rendement : changement de réactif, excès d’un réactif, élimination d’un produit  |
| * COM
 | Formuler et argumenter des réponses structurées Formuler et présenter une conclusion  |