The choice of conditions in industrial processes is based on a consideration of reaction rate, equilibrium yield and economic costs. While conditions such as high pressure and high temperature typically lead to faster reactions, they may decrease the yield of product. Such situations often involve a ‘compromise’ in reaction conditions. An understanding of factors related to reaction rates and equilibrium yield allow the particular conditions used in steam reforming, the synthesis of methanol and the Haber process to be better understood.

**Steam Reforming**

The purpose of steam reforming is to generate precursor substances for the Haber process and for the synthesis of methanol. This reaction can be represented with the following equation:

CH4(g) + H2O(ℓ) ⇌ CO(g) + 3 H2(g); ΔH = +ve

This reaction uses a moderate pressure of 10-20 atmospheres. The rate of formation of products would be increased with the use of a higher pressure due to more collisions between reactant particles. The yield, however, would decrease at higher pressures as increasing pressure would favour the side of the reaction with the least moles of gas (left-hand side). Also, high pressures are costly to operate and have safety risks. The moderate pressures used are therefore a compromise which allows for reasonable rate and yield of products at an acceptable cost.

The temperature used in this process is reasonably high. Reaction rates are increased at higher temperatures. This is because if particles have greater average kinetic energy then more particles will have energy greater than the activation energy and therefore a greater proportion of collisions will be successful. Additionally, the increased speed of particles means that collisions would be more frequent. High temperatures also favour yield in this reaction because increasing the temperature will favour the endothermic (forward) reaction. Heating to these temperatures is affordable, especially when re-using the heat given off by another chemical reaction (e.g. the exothermic synthesis of methanol or the Haber process). High temperatures therefore favour rate and yield with no economic disadvantage.

Steam reforming uses a nickel catalyst. The purpose of a catalyst is to increase reaction rate by providing an alternative reaction pathway with lower activation energy (Ea). This means that a greater proportion of particles will have energy greater than the catalysed Ea. Because catalysts increase forward and reverse rate equally, they have no effect on yield of product. Catalysts allow the reaction to occur at faster rates without further increasing temperature and pressure, which would have additional operating costs and safety risks. They are not consumed in the chemical reaction, which means they are reusable and therefore an an economically effective way of boosting reaction rate.

**Synthesis of methanol and ammonia**

Methanol (CH3OH) and ammonia (NH3) are synthesised by reactions of CO(g) and N2(g) with hydrogen, as shown in the equations below. Both reactions are exothermic.

Synthesis of methanol: CO(g) + 2 H2(g) ⇌ CH3OH(g); ΔH = -ve

Haber process: N2(g) + 3 H2(g) ⇌ 2 NH3(g); ΔH = -ve

The reaction conditions for these two reactions are compared in the following table. Although there are slight differences in the temperature and pressure conditions used, overall there is a high degree of similarity in the conditions used. Both reactions use catalysts to increase reaction rate, although the particular catalyst used for each reaction is different.

|  |  |  |
| --- | --- | --- |
| **Conditions** | **Synthesis of methanol** | **Haber process** |
| Temperature | 250 °C  (Moderate) | 400-450 °C  (Moderate) |
| Pressure | 50-100 atmospheres  (High) | 200 atmospheres  (High) |
| Catalyst | Cu / ZnO / Al2O3 | Iron-based |

Both reactions use moderate temperatures. Both of these reactions are exothermic, which means an increase in temperature will decrease the equilibrium yield of productions. The temperature cannot be too low, however, as decreasing temperature will slow the rate of forwards reaction due to particles having less kinetic energy. A moderate temperature is needed as a compromise between both rate and yield.

Both reactions use high pressures. Increasing the pressure will favour the side of the reaction with the least moles of gas, which in both reactions is the forward reaction. This means that high pressures will favour a greater yield of product. High pressures also favour reaction rate due to more collisions between particles. High pressures are costly to maintain, however, so this is why higher pressures are not used.

There are only minor differences between the temperature and pressure conditions used for each reaction. This may be due to differences in yield distribution or rates for each particular reaction. For example, the methanol reaction uses slightly lower temperatures and pressures than the Haber process reaction. This may mean that the synthesis of methanol occurs more readily than the synthesis of ammonia, and therefore does not need the same temperature and pressure conditions to proceed at an acceptable rate. In reality each reaction would be tested at different temperatures and pressures to find the optimum conditions for that reaction. These differences are only minor, however, and in general terms there is a high degree of similarity in the conditions used for each reaction.