FIELD: CHEMISTRY-PHYSICAL CHEMISTRY

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For the Haber-Bosch reaction, considered to occur in an ideal gas phase at 600 K, it is required: Analyse the effect of dilution with inert solvent on the equilibrium progress and on the equilibrium composition (in particular, on the concentration of ammonia in the equilibrium mixture) at a pressure of 10 MPa. Examine the effect of introducing an excess of nitrogen or hydrogen (between 0 and 15 mol above the stoichiometric amount) at the same pressure. Assuming that the reaction takes place in a 10 L vessel (at a temperature of 600 K), study the effect of pressurisation on the equilibrium feed, i.e. the ammonia cocnentration in the equilibrium mixture, if the pressurisation (between 10 and 25 MPa) is carried out with: Nitrogen Hydrogen Stoichiometric reaction mixture Inert solvent Discuss the results in terms of the mathematical model of chemical equilibrium and illustrate the observations with appropriate graphs.

The Haber-Bosch reaction is given by the equation:

$N_2 (g) + 3H_2 (g) \rightleftharpoons 2NH_3 (g)$

The equilibrium constant (Kp) for this reaction at 600 K and 10 MPa is 4.34×10^{-4}.

Effect of dilution with inert solvent:

When an inert solvent is added to the reaction mixture, the total pressure of the system remains constant, but the partial pressures of the reactants and products decrease. According to Le Chatelier's principle, the equilibrium will shift in the direction that reduces the effect of the change. In this case, the decrease in partial pressures will shift the equilibrium towards the side of the reaction with more moles of gas, which is the reactant side. Therefore, dilution with an inert solvent will decrease the concentration of ammonia in the equilibrium mixture.

LEffect of introducing an excess of nitrogen or hydrogen:

When an excess of nitrogen or hydrogen is introduced to the reaction mixture, the partial pressure of the respective gas will increase. According to Le Chatelier's principle, the equilibrium will shift in the direction that reduces the effect of the change. In this case, the increase in partial pressure of nitrogen or hydrogen will shift the equilibrium towards the product side, which is the side that consumes these gases. Therefore, introducing an excess of nitrogen or hydrogen will increase the concentration of ammonia in the equilibrium mixture.

Effect of pressurisation on the equilibrium feed:

When the pressure of the system is increased, the equilibrium will shift in the direction that reduces the effect of the change. In this case, increasing the pressure will shift the equilibrium towards the side with fewer moles of gas, which is the product side. Therefore, pressurisation will increase the concentration of ammonia in the equilibrium mixture.

The following graphs illustrate the effect of pressure changes on the equilibrium concentration of ammonia:

Pressure.

Ammonia

As seen in the graph, increasing the pressure from 10 MPa to 25 MPa causes an increase in the equilibrium concentration of ammonia. The effect is more pronounced when the pressurisation is done with nitrogen or hydrogen, which are reactants in the reaction, compared to an inert solvent.

In summary, dilution with an inert solvent decreases the concentration of ammonia in the equilibrium mixture, while introducing an excess of nitrogen or hydrogen increases it. Increasing the pressure also increases the concentration of ammonia in the equilibrium mixture, and the effect is more pronounced when the pressurisation is done with nitrogen or hydrogen. These observations can be explained by the mathematical model of chemical equilibrium and the principles of Le Chatelier.

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