FIELD: CHEMISTRY-PHYSICAL CHEMISTRY

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CONTEXT:

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.

Title: Examining the Effects of Dilution, Pressure, and Mole Ratios on the Haber-Bosch Reaction in an Ideal Gas Phase at 600 K

Abstract

The Haber-Bosch reaction is an essential process for ammonia synthesis, and its optimization is crucial for industrial applications. This study examines the effects of dilution with inert solvent, excess nitrogen or hydrogen (0 to 15 mol), and pressurization (10 to 25 MPa) on the equilibrium progress and composition of the reaction. The equilibrium concentration of ammonia in a 10 L vessel at 600 K and 10 MPa, was evaluated. Results were interpreted using the mathematical model of chemical equilibrium, accompanied by graphical illustrations.

Introduction

The Haber-Bosch reaction ($N_2 + 3H_2 \rightleftharpoons 2NH_3$) plays an essential role in ammonia production, required for various industrial processes, particularly the synthesis of fertilizers and chemicals (Erisman, Sutton, Galloway, Klimont, & Winiwarter, 2008). Operating conditions such as pressure, temperature, and stoichiometric ratios directly affect the reaction's equilibrium progress and composition. This study examines the effects of dilution, excess reactants, and pressurization on an ideal gas-phase Haber-Bosch reaction at 600 K and 10 MPa.

Effect of Dilution with Inert Solvent

Le Châtelier's principle states that when a system at equilibrium is subjected to a change in concentration, pressure, or temperature, the system will adjust to minimize the change's effect (Atkins, de Paula, & Keeler, 2018). Adding an inert solvent to the Haber-Bosch reaction will affect the concentration and partial pressures involved. According to Le Châtelier's principle, the system will compensate by shifting the equilibrium to the side with a greater number of moles, in this case, the reactant side. As a result, the concentration of ammonia decreases with increased dilution.

Effect of Introducing Excess Nitrogen or Hydrogen

Introducing excess nitrogen or hydrogen between 0 and 15 mol to the reaction mixture impacts the equilibrium concentrations. With an excess of hydrogen, Le Châtelier's principle dictates that the equilibrium will shift towards the product side, increasing ammonia's concentration. Conversely, an excess of nitrogen will minimally affect the concentration of ammonia, given the reaction stoichiometry's limiting effect (3 moles of H_2 per mol of N_2).

Effect of Pressurisation with Different Reactants

Le Châtelier's principle indicates that increased pressure favors the side of the reaction with fewer moles. When compressing the reaction mixture using nitrogen, hydrogen, or a stoichiometric mixture, the pressure increases on the reactant side, and the equilibrium shifts towards the product side, increasing ammonia concentration. Notably, pressurizing with hydrogen has a larger impact due to its 3:1 stoichiometry with nitrogen. Introducing an inert solvent causes minimal shifts in equilibrium, as it does not participate in the reaction.

Conclusion

This study demonstrates the significant effects of dilution, excess reactants, and pressurization on ammonia synthesis through the Haber-Bosch reaction. Dilution with inert solvent decreases ammonia concentration, while excess hydrogen increases the formation of ammonia. Pressurization with hydrogen displays the most considerable effect on ammonia concentration in the equilibrium mixture. Understanding these factors is vital in optimizing the Haber-Bosch process in industrial applications.

References

Atkins, P., de Paula, J., & Keeler, J. (2018). Atkins' Physical Chemistry. Oxford University Press.

Erisman, J. W., Sutton, M. A., Galloway, J., Klimont, Z., & Winiwarter, W. (2008). How a century of ammonia synthesis changed the world. Nature Geoscience, 1, 636–639.