CHEMISTRY
CHALLENGES AND SOLUTIONS

Control a Haber-Bosch Ammonia Plant Interactive Lab Lesson Plan

Introduction:
The *Control A Haber Bosch Ammonia Plant* simulation allows students to explore a practical example of an equilibrium reaction to see the effects of variables including temperature, pressure, and different catalysts. In this activity, learners optimize the profits generated by a simulated Haber-Bosch process ammonia fertilizer plant by trying to produce the largest daily output of ammonia as efficiently, and cost effectively, as possible.

In this simulation, the raw materials—nitrogen and hydrogen—are combined in a reaction chamber to produce ammonia. Variables that can be optimized include pressure, temperature, and catalysts of three different quality levels. Students can also alter the flow rate, the percentage of purge (to prevent the build-up of inert gases), and the degree of cooling of the reaction gases to liquify and remove the ammonia. After each 24-hour run, a set of output data will be displayed. Key outputs include ammonia yield, time to equilibrate, and total tonnage of ammonia produced during the day. Costs and net profit are also displayed. Using the accompanying worksheet, learners will be guided as they test variables in a controlled manner and graph their results.

Background: The Haber-Bosch process is currently the most common process for the artificial fixing of nitrogen to create nitrogen-based fertilizers. Worldwide, over 100 million tons of ammonia are produced by this method every year; in fact, over 1/3 of the world's population is alive today because of the process (Smil, 2001).

The method for combining hydrogen and nitrogen in the laboratory was first accomplished in 1909 by German chemist Fritz Haber, for which he received the 1918 Nobel Prize in Chemistry. Carl Bosch, a chemist at BASF, used Haber's methods and scaled up the process so that it could become the industrial basis for producing large quantities of ammonia.

Over the years, the process has been studied in detail, resulting in many refinements and improvements in the process. This interactive is based, in part, on data collected through analysis of a pilot ammonia synthesis plant operated by the Tennessee Valley Authority in the mid-20th century (Baddour, et al. 1965).

The raw materials for making ammonia fertilizer are readily available. Hydrogen can be generated from natural gas, and nitrogen is the largest component of the atmosphere. Central to the problem of creating ammonia are the strong triple bonds in the diatomic nitrogen molecule. Catalysts lower the molecules' activation energy so that these bonds can be broken, allowing the process to proceed faster. As the reactants enter the catalytic chamber, there are many more nitrogen and hydrogen molecules than ammonia molecules, a situation that, according to Le Chatelier's Principle, favors the forward reaction. As the reaction proceeds, the percentage of ammonia molecules increases, and this rising concentration tends to favor the reverse process. Normally, the process would reach equilibrium and stop at a fixed amount of ammonia. However, the gas is not stationary, and as the ammonia is produced, it is removed by the cooling process. This restores the original imbalance that favors the creation of more ammonia, and so more is created when the reactants in the closed loop are recirculated through the reaction chamber.

Connections to Chemistry Course: There are many connections between this interactive and the content in Chemistry: Challenges and Solutions. Some of the places where the interactive content is directly related are:

Unit 6, Section 9 – Percent Yield
Unit 7, Section 9 – Bond Enthalpies (Sidebar: "Nitrogen's Triple Bond")
Unit 9, Section 7 – Equilibrium

Unit 9, Section 8 – The Equilibrium Constant Expression
Unit 9, Section 9 – Le Chatelier's Principle
Unit 12, Section 2 – When Molecules Collide (rate of reaction)
Unit 12, Section 5 – Catalysts

Objectives:

- Understand the implications of a reversible reaction.
- Understand the effects of variables of temperature, pressure, and catalysts on this reaction.
- Apply Le Chatelier's Principle to a practical equilibrium problem.
- Experiment with additional variables to learn the effect on the equilibrium of changing the rate at which the reactants flow through the synthesis loop, purging some of the gas out of the system, and cooling the chilling chamber allowing the ammonia to condense.

Procedure:

1. Have students run the simulation without changing any of the variables to get baseline data (i.e., not a good yield). Students can check their results using the **See Results** button. They should take note of yield, time to equilibrate, and net profit.

2. Students then explore the pressure setting. They should try at least 3-5 different pressure settings and then graph Pressure vs. NH_3 yield to answer the following questions:

What happens to the yield when pressure is increased?
What happens to the reaction rate when pressure is increased?
Is there a pressure that is too high to run the reaction?

As pressure is increased, the system will favor the forward reaction, so the yield of ammonia increases. Higher pressure leads to more collisions between hydrogen and nitrogen molecules, resulting in a faster reaction. In fact, to obtain the most ammonia possible in the equilibrium mixture, the pressure needs to be as high as possible. But putting pressure too high can lead to a possible explosion.

3. Students should next explore the temperature setting. They should try at least 4-5 different temperature settings and then graph temperature vs NH_3 yield, to answer the following questions:

What happens to the yield when temperature is increased?
What happens to the reaction rate when temperature is increased?
Is there a temperature that is too low to run the reaction?

Overall, ammonia synthesis is an exothermic reaction, so increasing the temperature will tend to shift the equilibrium yield toward making less ammonia, rather than more. However, increasing the temperature makes up for this by increasing the rate of reaction, allowing more ammonia to be made, which can then be removed.

4. Next, students should keep other variables the same and try different catalyst settings to answer the following questions:

What happens to the yield when the catalysts are changed?
What happens to the reaction rate?

How does changing catalysts affect net profit?

5. Finally, students should try different runs to vary the settings of the other variables (flow rate, purge, and cooling), attempting to find the ideal conditions to make the largest profits. They should notice that some factors increase yield but also increase costs, thus reducing profits.

References:

Baddour, R. F., Brian, P. L. T., Logeais, B. A., & Eymery, J. P. (1965). Steady-state simulation of an ammonia synthesis converter. *Chemical Engineering Science*, 20(4), 281–292.

Smil, Vaclav. *Enriching the Earth: Fritz Haber, Carl Bosch, and the Transformation of World Food Production*. Cambridge, MA: The MIT Press (2001).