**Haber's Process - A computer Simulation**

**Introduction**

Haber's process is used to produce ammonia on an industrial scale.  Nitrogen and hydrogen in the gaseous phase are combined to produce ammonia according to the following equation:

                  N2 (g)   +  3 H2   (g)    <==>    2  NH3   (g)   **∆Hreaction**  =  - 92.38 kJ

In general the rate of a chemical reaction is increased with an increase in temperature, an increase in pressure, and the addition of a catalyst.

An increase in the pressure of an equilibrium system shifts the equilibrium in the direction of decreasing pressure.    Since in the above equation 1 volume of N2 and 3 volumes of H2combine to form 2 volumes of NH3 the pressure of the system would decrease if the reaction were to shift to the right.

**Procedure**

Go to the IB chemistry 1-2 or chemistry 1-2 web page and the spreadsheet file labeled Haber’s Process (Excel)

For purposes of this program you are to assume the roll of an industrial engineer.  You are in charge of production for an ammonia plant.  Your job is to produce ammonia as efficiently and as cheaply as possible.  You may alter the pressure and the temperature of your system as you wish.  You have choice of three catalysts: iron, tungsten, or platinum. If you choose you may use no catalyst at all.   Of the three catalysts,  iron is the least expensive. Platinum is by far the most expensive.

Your first goal is to maximize your percent yield of ammonia yet staying within a reasonable time frame for the reaction of a few minutes. The settings that you choose will for pressure, temperature and catalysts will determine your results.  Try several different settings and keep track of your settings, i.e. pressure, temperature, catalyst; and your results (time to equilibrium and yield)

Begin by trying several different pressures holding the temperature, and the choice of catalysts the same.  Repeat the procedure trying several different temperatures and holding the pressure and choice of catalysts constant.  Then hold the temperature and pressure constant while trying the four different catalyst choices; iron, tungsten, platinum or no catalyst at all.  Try to determine how the pressure temperature and the choice of catalysts each affect the yield.  Then choose the temperature pressure and catalyst combination that you think is best.  Try adjusting the variables up and down so as to increase the yield and shorten the time.

Your second goal is to manage production so as to generate a profit.  Profitability is determined by the efficiency with which you produce ammonia as well as economic factors such as the cost of energy, cost of producing

There are several independent variables that you can vary in this simulation and  essentially three dependent ones:  time to equilibrium, yield, and profit.   Be sure that you vary each of the independent variables over a range to find out how each one affects the results.  Then try several combinations of  variables to optimize your results.    After you have tried at least 10-15 (more if time permits) new combinations, determine your best choices and  discuss them in your recommendations .

.

**Report:**

* Record your 10  best scenarios.  Identify the conditions that are most optimal for the production of ammonia.  Keep in mind that both the yield and the time to come to equilibrium are important.
* Show using  your data , how varying temperature, pressure, and the use of catalysts influences  the dependent variables; yield and the  time to come to achieve equilibrium   Higher temperatures and pressures have higher costs associated with them as well.
* What criteria did you use to make your decision?
* Evaluate your results and write your conclusion and defend your position in a conclusion