Chem 120
Dr. Rusay

Group Equilibrium Lab

The lab grade will be based on your group's solution to the following equilibrium problem. 25 pts will be based on Dr. R's opinion of the solution, everyone receiving that grade, plus 5 pts from the other members of your group who will judge your contribution: (Unexcused absences will constitute a grade of 0.). Each group will provide a typed or **neatly** written summary of their recommendations to Dr. R.. The entire group must be prepared to fully explain the chemical basis for the group's recommendations.

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

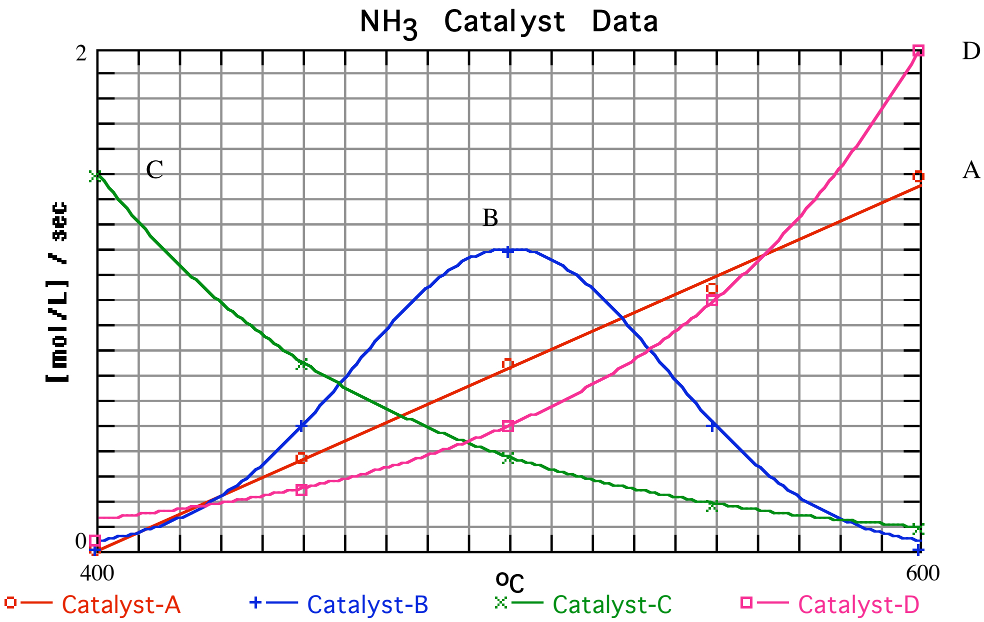
$$\Delta H^o_{rxn} = -92.2 kJ/mol\ @25^oC$$

The commercial production of ammonia from nitrogen (obtained from liquified air) and hydrogen (sourced from oil refineries or coal) began in Germany just prior to WW I. Germany needed explosives that could be made from ammonia or naturally occurring nitrates which were only available from India or Chile. Since Britain could easily interdict those natural supplies, 2 German scientists, Fritz Haber and Carl Bosch, were commissioned to find a chemical solution which they did. Haber's chemistry and Bosch's engineering resulted in 2 Nobel prizes for their accomplishments. Their process is still used today.

Approximately 30 billion pounds of ammonia are sold annually in the U.S. It is used primarily in agriculture as fertilizer. Since a fair amount is imported, a project feasibility study has been undertaken by E. N. Vyro Chemical Co., Inc., a U.S. firm. The engineering department developed a pilot plant design based on existing ammonia plants which has a continuous reactor that can be operated between 400-600 ºC and pressures of 100 to 300 atm. A rough plant design was developed which was based on production of at least 50,000 kg being produced each day using (2) eight hour shifts per day and a 5 day work week. Consider that high temperatures and pressures will cause reactor fatigue to occur much more rapidly than at lower levels. Also, the reactor's surface area and hence its size is to be as small as feasibly possible. These constraints will help reduce maintenance costs.

A critical part of E. N. Vyro's plan is to use one of several in-house proprietary catalysts which may offer a significant advantage over other competitive processes. The catalysts are all used in the same respective amounts, their chemistry is a company secret and their costs differ substantially: A=$50 / MT (Metric Ton NH_3 produced); B=$100 / MT; C=$150 / MT; D=$300 / MT. The catalysts do not perform outside of the temperature ranges noted in the accompanying graph.

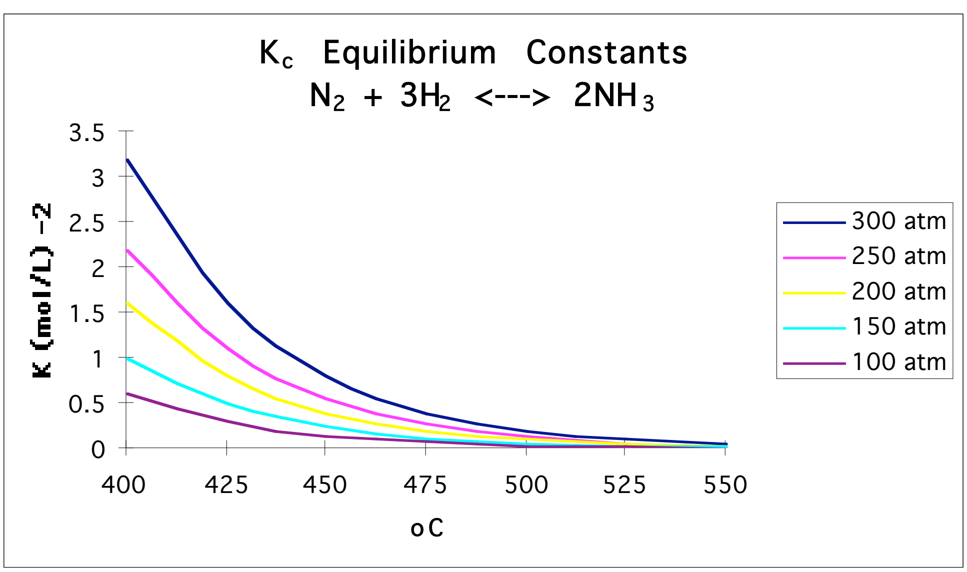
As the Company's chief R&D chemists you are to: (1) recommend a catalyst, and to define, (2) the size of the reaction vessel (Volume in Liters) (3) the operating pressure in atm (4) the operating temperature oC (5) the rate of addition (kg / sec) of the reactants, N_2 and H_2 and (6) the rate of condensation of NH_3 (kg / sec).



One concern raised by the marketing Vice President is NH_3's sales price, which is \$0.50/kg. A competitive fertilizer to NH_3 is ammonium nitrate which has an estimated minimum sales price of \$0.40/kg. Does the price difference affect the project?

Of course, as in in any big business decision (the full scale plant could cost more than \$50MM), the chairman, Dr. R., who fashions himself to be somewhat of an expert on equilibrium processes, plans to personally review your recommendations. Your group should be prepared to address his questions on equilibria and defend the logic behind your recommendations. Your recommendations must also address the market challenge of ammonium nitrate, i.e., a selling price that is \$0.10/kg less than ammonia.

As you are well aware, nitrogen and hydrogen do not react at room temperature, and higher temperatures do not favor formation of ammonia since the Equilibrium constant decreases with increased temperature.



The following schematic satisfies the engineering. You have been asked to solve the chemical problem just as Haber had been. Some advice is to begin with the rates of reaction for the different catalysts and apply Le Chatelier's principle.

$$K_p = K_c (RT)^{\Delta n}$$

Approach the challenge stepwise with a critical approach.... i.e. Define what are the critical features: Quantity?, Concentration?, T?, P?, K?, Rates of Reaction?, Costs? 1.) Which feature is most important in the problem? (Fix your aim on it!) 2.) What factors impact the main objective? 3.) How are they inter-related? 4.) Which one has the highest effect on the others? (Focus on it and fix values for it. Repeat step 4.) etc. until there is only one parameter left to satisfy.