Activity 3: Planning an Investigation

You are working as a chemical engineering consultant to solve a design problem for Haber Manufacturing, an ammonia (NH_3) production facility. They have given you 180-day access to one of their production lines to conduct a pilot study. Your objective is to determine the conditions that lead to the highest daily yield of ammonia. Haber Manufacturing synthesizes NH_3 by the reaction

$$N_{2(g)} + 3\ H_{2(g)} \leftrightarrows 2\ NH_{3(g)}$$

The reaction is reversible and has a ΔH of -92.4 kJ.

The production facility uses a **continuous flow process** as opposed to a batch process. Raw materials flow into the reactor on a continuous basis and react while they flow from the entry point to the exit point. For this reason, it is critically important that the reaction occur relatively fast, before the gases reach the end of the production line.

There are four input parameters to consider in your pilot study:

- Reactor Temperature (ranges from 0°C to 1500°C)
- Reactor Pressure (ranges from 1 atm to 1500 atm)
- N_2 Flow Rate (ranges from 0 L/min to 200 L/min)
- H_2 Flow Rate (ranges from 0 L/min to 200 L/min)

Haber will provide a daily report that identifies five output parameters. They are

- Percent Yield (averaged for that day)
- Daily Yield of NH_3 (in kg)
- Daily Profit (in $, indexed to fixed costs of raw materials and NH_3 sale price)
- Carbon Rating (1 – 100; based on electrical costs*)
- Safety Rating (1 – 100; based on reactor temperature and pressure)

Besides the Equilibrium model for reversible reactions, you will also need to consider three additional models:

Stoichiometry:	The coefficients in the balanced chemical equation indicate the ratio of N_2 to H_2 required by the reaction.
Kinetics:	Reaction rates are greater at higher temperatures compared to lower temperatures. Reaction rates also increase with increasing concentrations.
Thermodynamics:	Substances such as NH_3 are less stable at high temperatures and tend to decompose more rapidly when exposed to excessively high temperatures.

* The NH_3 production process does not directly produce ammonia. The Carbon Rating is tied to electrical power generation which relies on combustion of natural gas.

Activity 4: Refining the Design

Your project team has taken over the operation of Production Line 12 at the ammonia production plant. Each day, you run the line with a different set of parameter values. You carefully record the input parameters – reactor temperature, reactor pressure, N_2 flow rate, and H_2 flow rate. By day's end, you receive a report identifying the average % yield value, the amount of NH_3 produced, the company profits, and a carbon rating and risk rating.

Your team is making steady progress towards the goal: determining the conditions that lead to the greatest daily NH_3 production. Making such progress demands careful analysis of the data and good decision-making. In this activity, you will demonstrate your ability to analyze the data to make decisions that optimize the amount of NH_3 production.

Activity 5: Board Meeting

As the end of the 180-day pilot study approaches, your project team is preparing for their presentation to the Board of Directors of Haber Manufacturing. In the presentation, you will identify the conditions that result in the greatest daily production of NH_3 and provide supporting evidence and reasoning for your claim. You will also present some of the trade-offs associated with operating the production line at such high temperature and pressure conditions. The presentation will center around the use of a Slide Deck with your claims and evidence.The Board will have questions after your presentation. You will need to be prepared for the most difficult questions