Worksheet: Chemical equilibrium

Name(s) ________________________________

This experiment uses gas-phase equilibrium concentrations for the ammonia formation reaction to determine the equilibrium constant. The heat of reaction is determined by measuring the equilibrium constant over a range of temperatures.

Student learning objectives

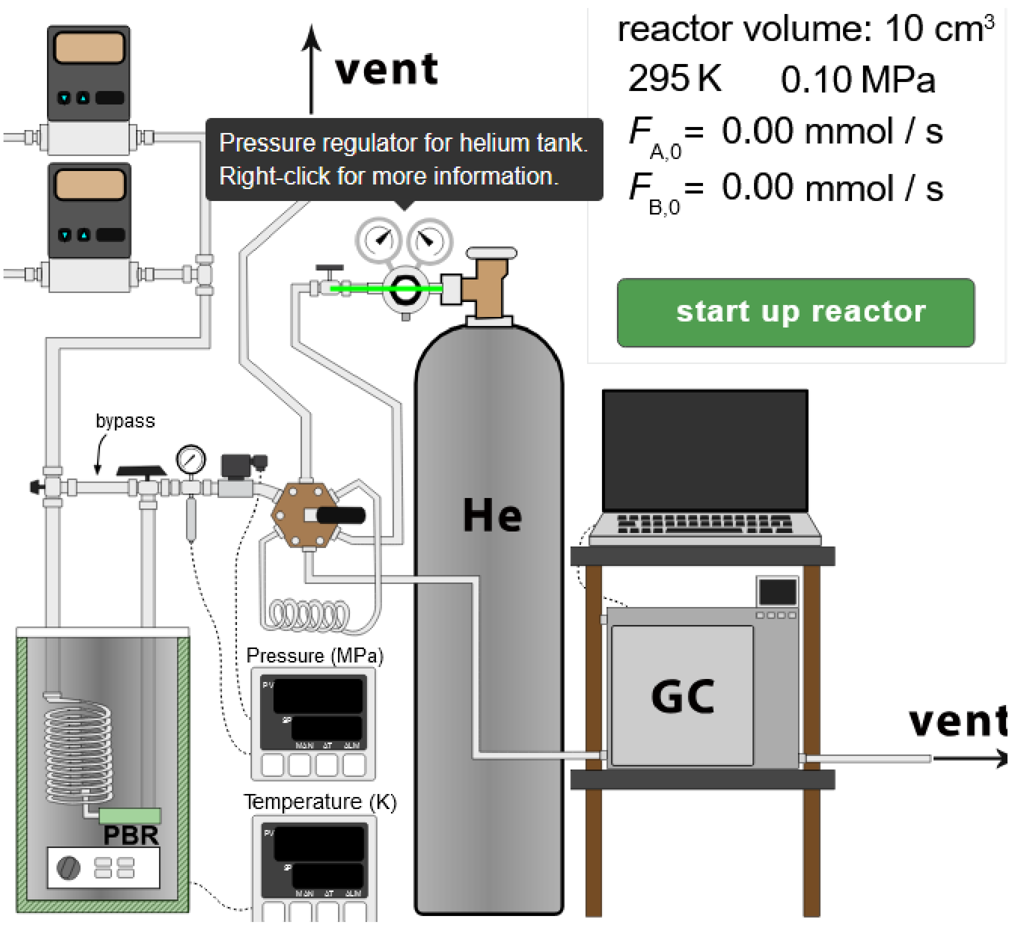
1. Be able to calculate an equilibrium constant from equilibrium concentrations.
2. Be able apply the van Hoff equation to determine the heat of reaction.

Equipment

Maybe use a modified version of this from the Virtual Catalytic Reactor Laboratory

Modify so it is a closed recirculating loop with a pump to move the gas around, a sampling valve and a He tank for sampling, and a GC.

The packed bed reactor contains a catalyst.



Questions to answer before starting the experiment

How does the equilibrium constant change with temperature for an exothermic reaction? Explain.

How does the equilibrium constant change with a change in pressure for a gas-phase reaction?

What are the units of an equilibrium constant?

Before starting

The gas-phase reaction, which is conducted commercially at high temperature and high pressure, is catalytic formation of ammonia.

$N_2 + 3\ H_2 \rightarrow 2\ NH_3$

Procedure: look at the VCRL for ideas

1. Start the recirculating pump.
2. Turn on the sand bath heater and set the temperature.
3. Allow time for the system to reach equilibrium.
4. Take a sample and inject into the GC using the sampling valve.
5. Wait and take another sample and inject into the GC.
6. If the composition has not changed, then assume the system is at equilibrium.

Record temperature, pressure, and mole fractions. Calculate partial pressures and enter in the table.

		Mole fraction			Partial pressure (bar)			
Temperature (K)	Pressure (bar)	N_2	H_2	NH_3	N_2	H_2	NH_3	K

Calculate the equilibrium constant.

$$K_{eq} = \frac{\left(\frac{P_{NH3}}{1\ bar}\right)^2}{\left(\frac{P_{H2}}{1\ bar}\right)^3 \left(\frac{P_{N2}}{1\ bar}\right)}$$

In this equation, the pressure is in units of bar, and the equation is usually written as indicated below, where the pressure must be in bar and the equilibrium constant is dimensionless.

$$K_{eq} = \frac{P_{NH3}^2}{P_{N2} P_{H2}^3}$$

This equation assumes ideal gases, which is not correct at the high pressures used for ammonia formation but is used here to make the calculations easier.

Repeat this measurement at the same temperature but at different pressures in the range and record in the table.

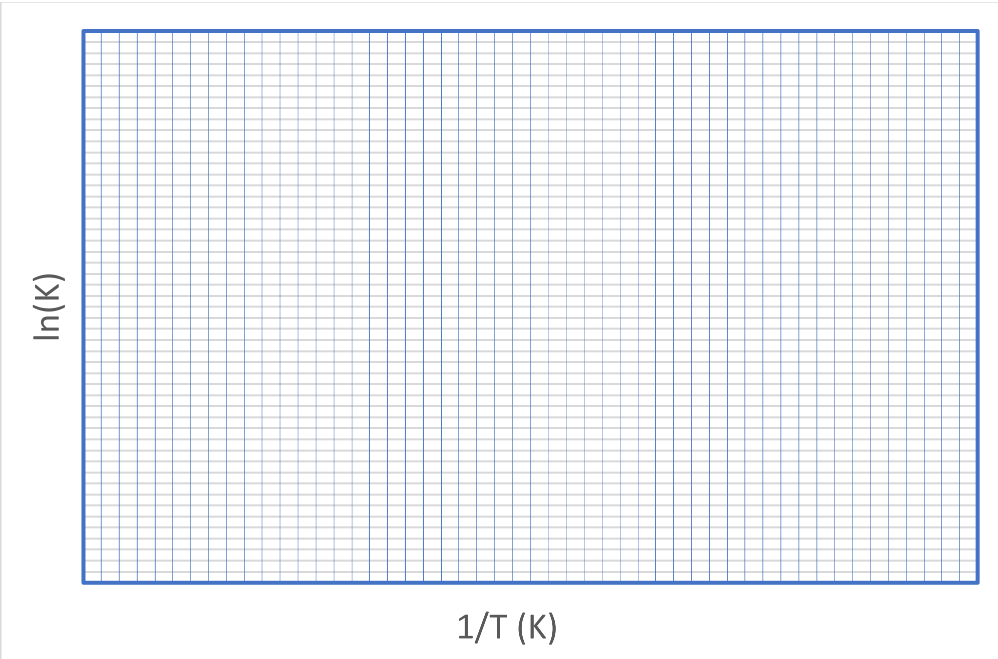
What can you conclude about the effect of pressure on the equilibrium constant?

Measure equilibrium compositions at a range of temperatures and calculate the equilibrium constant at each temperature. Record the values in the table below.

		Mole fraction			Partial pressure (bar)			
Temperature (K)	Pressure (bar)	N_2	H_2	NH_3	N_2	H_2	NH_3	K

Data Analysis:

Plot ln(K) versus inverse temperature.



Can the data be fit by a straight line?

Calculate the heat of reaction from the van Hoff equation, using all your data.

$$\ln\left(\frac{K_2}{K_1}\right) = -\frac{\Delta H_{rxn}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

where K_2 (dimensionless) is the equilibrium constant at temperature T_2

K_1 (dimensionless) is the equilibrium constant at temperature T_1

T_1 and T_2 are absolute temperatures (K)

ΔH_{rxn} = heat of reaction (J/mol)

R = ideal gas constant (J/mol K)

ΔH_{rxn} = _________ J/mol = _________ kJ/mol

Questions to answer

1. Where might these measurement have errors?

2. What safety precautions would you take to conduct this experiment in the laboratory?