EXTENSION ACTIVITY INTRODUCTION TO COLLEGE CHEMISTRY

LECHÂTELIER KEY

Activity Directions

This activity will serve as practice for the topics covered in the LeChâtelier game. This activity is best used in conjunction with not only the tutorial levels, but also supplementary learning resources such as course lectures, textbook reading, etc. Questions labeled "Lock It In" are simply opportunities for you to solidify what you have accomplished in each task and help ensure you meet each objective. 1. Log into Collisions and navigate to the LeChâtelier Game.

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- 2. Play the Tutorial levels, if you haven't done so already.
- 3. Exit the levels and enter the LeChâtelier sandbox.
- 4. Follow all instructions as written below. Be sure to reference your course's textbook, lecture notes, etc. as needed.



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Demonstrate how to calculate the equilibrium constant in terms of concentration (K_c) for a reaction and use it to determine if the forward or reverse reaction is favored.

It has long been noticed that reactions often do not go to completion in the way that is predicted by stoichiometric ratios. A mixture of two reactants in an ideal ratio do not necessarily convert entirely to products. We now know that many chemical reactions are actually reversible in that the reaction that converts reactant molecules into products simultaneously occurs in reverse to convert products back into reactants. These reactions can happen at different rates depending on the conditions, but they will eventually reach a state of **dynamic equilibrium** in which the forward and reverse reactions are occurring at the same rate. You should have noticed that the reactions in the LeChâtelier game never stop occurring. Instead, eventually the rate at which you see products appearing is the same as the rate at which you see reactants reappearing.

Try going to the sandbox to see this in action again. You should notice that the rate counters above the reaction chamber are equal. The reaction is at a state of dynamic equilibrium. Now try to use the toggle beneath the chamber to filter your view to look only at the reactants. Then do the same to look only at the products. It should be clear to you that although the rates are equal, the concentrations of reactants and products are typically not. It is very important that you remember this distinction.

The fact that concentrations are not necessarily equal at equilibrium does not mean that there is no means of making sense of equilibrium concentrations. At a given temperature, the concentrations of reactants and products at equilibrium in a reversible reaction will always have the ratio of the product of the equilibrium concentrations of the reactants raised to their stoichiometric coefficients to the equilibrium constant (K) and the relationship is known as the **law of mass action**. Consider the following reaction at 300 Kelvin:

$\mathbf{aA} + \mathbf{bB} \rightleftharpoons \mathbf{cC} + \mathbf{dD}$

The value of K in terms of concentration (K_c) for this reaction in the forward direction would be determined by the following expression:

$$\mathsf{K}_{c} = \frac{[\mathsf{C}]^{c} [\mathsf{D}]^{d}}{[\mathsf{A}]^{a} [\mathsf{B}]^{b}}$$

[] = Molar Concentration in (Moles/Liter)



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Demonstrate how to calculate the equilibrium constant in terms of concentration (K_c) for a reaction and use it to determine if the forward or reverse reaction is favored.

The equilibrium constant (K) has a few very important characteristics:

- 1. Its value is specific to the reaction of interest at one particular temperature.
- 2. Neither concentration nor pressure affect the value of K.
- 3. Despite different initial concentrations of reactants and products leading to different final concentrations at equilibrium, the value of Kc remains unchanged. All final concentrations will be at a ratio equivalent to K₂.
- 4. Changes in temperature will change the value of K.

Since our reaction is reversible, it is important to realize that the K for the reverse reaction is simply the inverse of the K for the forward reaction ($\frac{1}{\kappa}$). It is often identified as K'.

TASK 1: Write out the equilibrium constant expression in terms of concentration for each of the homogenous forward reactions (K_c) from the sandbox listed in the table below. In the third column, write the equilibrium constant expression for the reverse reaction (K_c). The first one has been done for you.

Reaction	Forward Reaction Equilibrium Constant Expression (<i>K</i> _c)	Reverse Reaction Equilibrium Constant Expression (<i>K</i> _c ')
$2 \text{ CO}(g) + O_2(g) \rightleftharpoons 2 \text{ CO}_2(g)$	$K_{c} = \frac{[CO_{2}]^{2}}{[CO]^{2} [O_{2}]}$	$K_{c}^{T} = \frac{[CO]^{2} [O_{2}]}{[CO_{2}]^{2}}$
$H_2(g)$ + $Cl_2(g) \rightleftharpoons 2$ HCI (g)	$K_{c} = \frac{[HCI]^{2}}{[H_{2}][CI_{2}]}$	$K_{c}^{\dagger} = \frac{[H_{2}][CI_{2}]}{[HCI]^{2}}$
CO (g) + 3H₂(g) ⇔ CH₄(g) + H₂O (g)	$K_{c} = \frac{[CH_{4}][H_{2}O]}{[H_{2}]^{3}[CO]}$	$K_{c}^{T} = \frac{[H_{2}]^{3}[CO]}{[CH_{4}][H_{2}O]}$
$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$	$K_{c} = \frac{[NH_{3}]^{2}}{[N_{2}][H_{2}]^{3}}$	$K_{c}^{'} = \frac{[N_{2}][H_{2}]^{3}}{[NH_{3}]^{2}}$

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Demonstrate how to calculate the equilibrium constant in terms of concentration (K_c) for a reaction and use it to determine if the forward or reverse reaction is favored.

LOCK IT IN:

What is the relationship between the equilibrium constants for the forward and reverse reactions? The equilibrium constant for the reverse reaction is the inverse of the forward reaction. This means it is only necessary to switch the contents of the numerator and denominator to determine the equilibrium constant of the reaction in the opposite direction.

Notice that all of the reactants in products that you saw in Task 1 were in the gaseous state. Since all of the reactants were in the same state of matter, they are said to be **homogeneous reactions**. However, many reactions will not be homogeneous and will occur between substances in different states of matter. Such reactions are classified as **heterogeneous**.

The distinction between these reactions is important because the equilibrium expression of heterogeneous reactions will only include substances in certain states. Since the concentration of pure solids and pure liquids only depend on their density, their concentrations do not change over the course of a heterogeneous reaction. As such, solids ('s' in the chemical equation) and liquids (' ℓ ' in the chemical equation) are **NOT** included in the equilibrium expression of a heterogeneous reaction.

Only substances identified as being in the gaseous ('g' in the chemical equation) or aqueous ('aq' in the chemical equation) states are included.



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TASK 2: Write the equilibrium constant expression for each of the heterogeneous forward reactions listed in the table below. In the third column, write the equilibrium constant expression for the reverse reaction. The first two are available to you in the sandbox.

Reaction	Forward Reaction Equilibrium Constant Expression (<i>K</i>)	Reverse Reaction Equilibrium Constant Expression (<i>K'</i>)
AgCl (s)	K _c = [Ag⁺][Cl⁻]	K _c ['] = <u>1</u> [Ag ⁺][Cl ⁻]
HCl (aq) + H₂O (ℓ)	$K_{c} = \frac{[H_{3}O^{+}][CI^{-}]}{[HCI]}$	$K_{c}^{T} = \frac{[HCI]}{[H_{3}O^{+}][CI^{-}]}$
Fe₃O₄ (s) + 4 H₂ (g) ≓ 3 Fe (s) + 4 H₂O (g)	$K_{c} = \frac{[H_{2}O]^{4}}{[H_{2}]^{4}}$	$K_{c}' = \frac{[H_{2}]^{4}}{[H_{2}O]^{4}}$
Cu (s) + 2 Ag⁺ (aq) ≑ Cu²⁺ (aq) + 2 Ag (s)	$K_{c} = \frac{[Cu^{2+}]}{[Ag^{+}]^{2}}$	$K_{c}^{'} = \frac{[Ag^{+}]^{2}}{[Cu^{2+}]}$

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Demonstrate how to calculate the equilibrium constant in terms of concentration (K_c) for a reaction and use it to determine if the forward or reverse reaction is favored.

The equilibrium constant is useful for many reasons, one of which is that it can help us determine how far a reaction will proceed at a particular temperature.

In some reactions, the products are heavily favored. In such a case, there are many more product molecules at equilibrium than reactant molecules. If we consider the structure of an equilibrium expression, a case in which the product molecules are far more abundant than reactant molecules at equilibrium would cause the numerator of the expression to be much larger than the denominator. In this case, the K_c would be much greater than 1. Since the K_c of the reverse reaction is simply the inverse of that of the forward reaction, the K_c of the reverse reaction in such cases would be very small.

In other reactions, the reactants are heavily favored. In these cases, very few of the reactant molecules are converted into product ones. The equilibrium expression in this case would have a much smaller numerator than the denominator. As such, K_c would be a value much smaller than 1. The opposite would be true of the reverse reaction.

There are many reactions, however, where the equilibrium is defined by similar concentrations of reactants and products. In these cases, K_{c} would be a value somewhere around 1.

Overall, K_c can range from very small numbers in which the forward reaction is relatively unfavorable to extremely large numbers in which the forward reaction is very favorable. Due to the extreme scales to which K_c can reach, you will often see them presented in scientific notation.

K _c	Result
K _c >> 1	Forward reaction progresses very far; reverse reaction does not progress far.
K _c ≈1	Forward and reverse reactions progress to similar degrees.
K _c << 1	Forward reaction does not progress far; reverse reaction progresses far.



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Demonstrate how to calculate the equilibrium constant in terms of concentration (K_c) for a reaction and use it to determine if the forward or reverse reaction is favored.

TASK 3: The equilibrium constant at 300 K for four of the sandbox reactions are listed below. Rank these reactions where the forward reaction that will proceed the farthest is at the top and the one where the forward reaction will proceed the least at the bottom.

Forward Reaction Proceeds Farthest	$H_2\left(g ight)+Cl_2\left(g ight) \rightleftharpoons 2 \ HCl\left(g ight)$
	$N_2(g)$ + 3 $H_2(g)$ \rightleftharpoons 2 $NH_3(g)$
	$H_2\left(g ight) + I_2\left(g ight) \rightleftharpoons 2 \;HI\left(g ight)$
Forward Reaction Proceeds Least	$2 \operatorname{NO}_2(g) \rightleftharpoons 2 \operatorname{NO}(g) + \operatorname{O}_2(g)$

LOCK IT IN: How would this ranking change for the reverse reactions?

Since the value of K_c for the reverse reaction is simply the inverse of the value of the forward reaction, the ranking would be flipped.



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A useful tool when dealing with equilibrium concentrations is called an **ICE** table. The **"I"** stands for **initial** concentration, the **"C"** for **change**, and the **"E"** for **equilibrium** concentration. Let's see how these tables can be used to analyze a scenario.

Consider the following reaction given that initially [A] = 1.00, [B] = 0.5, and [C] = 0.0, but at equilibrium [A] = 0.6.

$2A + B \rightarrow 2C$

An ICE table can be used to organize the given concentrations and then determine any missing concentrations.

	[A]	[B]	[C]
Initial 1.00		0.5	0.0
Change			
Equilibrium	0.6		

Using our understanding of stoichiometry, we know that any change in [A] will result in half of that change in [B] because of the 2:1 ratio of the coefficients. We also know that the ratio of the coefficients for A and C are 1:1 but opposite in direction—a decrease in [A] will lead to an increase of the same magnitude in [C]. Using this knowledge, we can complete the rest of the table.

	[A]	[B]	[C]
Initial	1.00	0.5	0.0
Change	-0.4	-0.2	+0.4
Equilibrium	0.6	0.3	0.4

Now that we know the equilibrium concentrations, we can calculate the value of K_{c} .

$$K_{\rm c} = \frac{[0.4]^2}{[0.6]^2 [0.3]} = 4.94$$



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TASK 4: The following sandbox reaction occurs at certain temperature:

$$CO(g) + 3 H_2(g) = CH_4(g) + H_2O(g)$$

The reaction mixture initially contains **[CO] = 0.5 M**, **[H**₂**] = 1.5 M**, **[CH**₄**] = 0.0 M**, and **[H**₂**O] = 0.01 M**. At equilibrium **[CO] = 0.01 M**. Determine the equilibrium constant of the reaction using an ICE table to two significant figures in scientific notation. Use the example problem to help you fill in the column labels and complete the problem. Write your final answer in the box beneath the table.

	[CO]	[H ₂]	[CH ₄]	[H ₂ O]
Initial	0.5	1.5	0.0	0.0
Change	- 0.49	- 1.47	+ 0.49	+ 0.49
Equilibrium	0.01	0.03	0.49	0.49

$$K_{c} = 8.9 \times 10^{5}$$



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Demonstrate an understanding of how changes in concentration, pressure, and temperature affect equilibrium according to LeChâtelier's Principle.

The central concept (and namesake) of the LeChâtelier Game is LeChâtelier's Principle named after the French chemist Henry Louis LeChâtelier. LeChâtelier realized that when a system is at equilibrium, it will respond to changes in concentration, temperature, and pressure to establish a new equilibrium in a way that works to counteract the change that occurred. Although you can find more detail in your textbook or lecture notes, the way reactions at equilibrium change in response to concentration, pressure, and temperature is summarized in the table:

Disturbance	Effect	Example	Reaction will shift towards
	An increase in concentration shifts	The concentration of a product is increased.	reactants.
	would counter that change.	The concentration of a reactant is increased.	products.
Concentration	A decrease in concentration shifts a reaction towards the substance	The concentration of a product is decreased.	products.
	decreased.	The concentration of a reactant is decreased.	reactants.
Partial Pressure	An increase in partial pressures shifts the reaction towards the side with the fewer moles of gas.	The partial pressures of the gases in a reaction are increased in a reaction where the reactant side has more moles of gas.	products.
		The partial pressures of the gases in a reaction are increased in a reaction where the product side has more moles of gas.	reactants.
		The partial pressures of the gases in a reaction are increased in a reaction where both sides have the same number of moles of gas.	neither side.



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Demonstrate an understanding of how changes in concentration, pressure, and temperature affect equilibrium according to LeChâtelier's Principle.

Partial Pressure (continued)	A decrease in partial pressures shifts the reaction towards the side	The partial pressures of the gases in a reaction are decreased in a reaction where the reactant side has more moles of gas.	reactants.
	with more moles of gas.	The partial pressures of the gases in a reaction are decreased in a reaction where the product side has more moles of gas.	products.
Temperature	An increase in temperature will shift the reaction towards the products in an endothermic reaction and towards the reactants in an exothermic reaction.	The temperature of an endothermic reaction is increased.	products.
		The temperature of an exothermic reaction is increased.	reactants.
	A decrease in temperature will shift the reaction towards the reactants in an endothermic	The temperature of an endothermic reaction is decreased.	reactants.
	in an exothermic reaction.	The temperature of an exothermic reaction is decreased.	products.





LECHÂTELIER - EXTENSION ACTIVITY - KEY





Demonstrate an understanding of how changes in concentration, pressure, and temperature affect equilibrium according to LeChâtelier's Principle.

TASK 5: Predict how the concentration disturbance listed for each reaction will affect the equilibrium of the reaction by determining whether the reaction will shift towards the **reactants** or **products**. After making your predictions, test them out using the sandbox.

Reaction	Enthalpy of Reaction/∆H _{rxn} (kJ/mol)	Concentration Disturbance	Reaction will shift towards… (reactants or products?)	Justification
$N_2(g)$ + 3 $H_2(g) \rightleftharpoons 2NH_3(g)$	-92	$[NH_3]$ increases	Reactants	An increase in the concentration of the products will shift a reaction towards the reactants.
$H_2\left(g ight)+I_2\left(g ight) \rightleftharpoons 2\;HI\left(g ight)$	-9.5	[l ₂] decreases	Reactants	A decrease in the concentration of a reactant will shift the reaction to produce more of it. That means that this reaction will shift towards the reactants.
$2 \operatorname{SO}_3(g) \rightleftharpoons 2 \operatorname{SO}_2(g) + \operatorname{O}_2(g)$	+198	[SO ₃] increases	Products	An increase in the concentration of the reactants will shift the reaction towards the products.

LOCK IT IN:

Explain why the pressure of the first reaction increased when you increased the concentration of ammonia (NH₃).



The pressure of the reaction increased in the first reaction because it shifted towards the products, which generates more moles of gas (four versus two). An increase in the number of moles of gas in the reaction chamber without a change in volume leads to an increase in the pressure.



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Demonstrate an understanding of how changes in concentration, pressure, and temperature affect equilibrium according to LeChâtelier's Principle.

TASK 6: Predict how the pressure disturbance listed for each reaction will affect the equilibrium of the reaction by determining whether the reaction will shift towards the **reactants** or **products**. After making your predictions, test them out using the sandbox.

Reaction	Enthalpy of Reaction/∆H _{rxn} (kJ/mol)	Partial Pressure Disturbance	Reaction will shift towards… (reactants, products, or neither?)	Justification	
CO (g) + 3H₂(g) ⇔ CH₄(g) + H₂O (g)	-206	All partial pressures increase.	Products	An increase in pressure will shift the reaction to the side with fewer moles of gas. In this case, there are four moles of reactants to only two moles of gas of products, so the reaction shifts to the products.	
$N_2(g)$ + 3 $H_2(g) pprox 2NH_3(g)$	-91	All partial pressures increase.	Products	An increase in pressure will shift the reaction to the side with fewer moles of gas. In this case, there are four moles of reactants to only two moles of gas of products, so the reaction shifts to the products.	
$2 \operatorname{SO}_3(g) \rightleftharpoons 2 \operatorname{SO}_2(g) + \operatorname{O}_2(g)$	+198	All partial pressures decrease.	Products	A decrease in pressure will shift the reaction to the side with more moles of gas. In this case, there are two moles of gas of the reactants to three moles of gas of products so the reaction shifts to the products.	
H ₂ (g) + Cl ₂ (g) ≑ 2 HCl (g)	-185	All partial pressures decrease.	No Change	A decrease in pressure will shift the reaction to the side with more moles of gas. However, the number of moles of gas is the same on both sides of the reaction, so there will be no	

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Demonstrate an understanding of how changes in concentration, pressure, and temperature affect equilibrium according to LeChâtelier's Principle.

LOCK IT IN:

What method does the sandbox use to increase the partial pressures of the reaction? Explain why this works.

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Boyle's Law tells us that pressure and volume are inversely related. Accordingly, the sandbox increases the partial pressures of the reaction by decreasing the volume of the reaction chamber.

LOCK IT IN:

Under what circumstances does pressure have no effect on the equilibrium of the reaction?



Pressure has no effect on the equilibrium of the reaction when the number of moles of gas is the same on both sides of the reaction.

LOCK IT IN: Explain why the **temperature** of the first reaction increased when

you increased the pressure.



The temperature of the reaction chamber increased because an exothermic reaction was shifted towards the products. In an exothermic reaction, heat can be treated as a product of the reaction, so when the reaction is shifted towards the products, the temperature will increase. It is important to note, however, that this temperature change will have an effect on the equilibrium of the reaction as well.



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Demonstrate an understanding of how changes in concentration, pressure, and temperature affect equilibrium according to LeChâtelier's Principle.

TASK 7: Predict how the temperature disturbance listed for each reaction will affect the equilibrium of the reaction by determining if the value K_c will **increase, decrease**, or remain **unchanged**. Then determine whether the reaction will shift towards the reactants or products. After making your predictions, test them out using the sandbox.

Reaction	Enthalpy of Reaction/∆H _{rxn} (kJ/mol)	Temperature Disturbance	Change in K _c (increase, decrease, unchanged?)	Reaction will shift towards… (reactants or products?)	Justification
2 NO ₂	+114	The temperature of the reaction increases.	Increase	Products	The positive enthalpy tells us that the reaction is endothermic. Increasing the temperature of an endothermic reaction shifts the reaction towards the products.
H₂ (g) + Cl₂ (g) ≓ 2 HCl (g)	-185	The temperature of the reaction increases.	Decrease	Reactants	The negative enthalpy tells us that the reaction is exothermic. Increasing the temperature of an exothermic reaction shifts the reaction towards the reactants.
2 SO ₃ (g) \rightleftharpoons 2 SO ₂ (g) + O ₂ (g)	+198	The temperature of the reaction decreases.	Decrease	Reactants	The positive enthalpy tells us that the reaction is endothermic. Decreasing the temperature of an endothermic reaction shifts the reaction towards the reactants.
CO (g) + 3H₂(g) ≓ CH₄(g) + H₂O (g)	-206	The temperature of the reaction decreases.	Increase	Products	The negative enthalpy tells us that the reaction is exothermic. Decreasing the temperature of an exothermic reaction shifts the reaction towards the products.



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Demonstrate an understanding of how changes in concentration, pressure, and temperature affect equilibrium according to LeChâtelier's Principle.

LOCK IT IN: Explain why the **pressure** of the first reaction increased when you increased the temperature. In to th th

Increasing the temperature of the endothermic reaction shifted it towards the products. Since there are more moles of gaseous product than reactant due to the stoichiometry of the reaction, a shift towards the products increases the pressure.

There are two special circumstances that are worth considering in the context of LeChâtelier— inert gases and catalysts. Although both seem as if they could affect the equilibrium of reaction, neither one does.

The addition of an inert gas to a reaction at a constant volume will certainly increase the pressure at which the reaction is occurring. It is important to remember, however, that the overall pressure of the reaction does not affect equilibrium. The partial pressures of each gas, however, do. Addition of a gas that will not be involved in the reaction should not change the equilibrium. The addition of a catalyst works to increase the rate of reaction in both directions. The key, however, is that the catalyst increases the rate of the forward and reverse reactions to the same degree. As a result, equilibrium is unaffected.

TASK 8: Predict how the special disturbances (inert gases and catalysts) listed for each reaction will affect the equilibrium of the reaction by determining if the value K_c will **increase**, **decrease**, or remain **unchanged**.

Reaction	Enthalpy of Reaction/∆H _{rxn} (kJ/mol)	Disturbance	Change in K _c (increase, decrease, unchanged?)	Reaction will shift towards (reactants, products, or neither?)	Justification
H₂ (g) + Cl₂ (g) ≈ 2 HCl (g)	-185	Helium gas is added to a reaction vessel at a constant volume so that the total pressure triples.	Unchanged	Neither	Addition of the helium only increases the total pressure of the reaction, but not the partial pressures of the reactants. As such, the equilibrium is unchanged.
$N_2(g)$ + 3 $H_2(g) pprox 2NH_3(g)$	-91	A catalyst is added to the reaction.	Unchanged	Neither	Addition of the catalyst increases the rate of the forward and reverse reactions equally. As such, the equilibrium is unchanged.



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CLOSURE

CLOSURE: One of the reactions available to you in the sandbox is part of what is certainly one of the most famous processes in chemistry— the Haber-Bosch Process. Due to the strength of the triple bond in the diatomic nitrogen found in the atmosphere, it is a rather inert substance. The Haber-Bosch process, however, is an extremely important industrial reaction that is able to hydrogenate the inert nitrogen to create ammonia.

 N_2 (g) + 3H₂ (g) = 2NH₃ (g) ΔH = − 91.8 kJ mol⁻¹

The ammonia produced in this reaction is primarily used to synthesize the chemical fertilizers that support much of modern agriculture. As such, chemical engineers have developed ways to increase the amount of ammonia that they are able to produce from the reaction. Use what you have learned in this extension activity to write a paragraph or several bullet points explaining the factors that a chemical engineer would want to consider and/or implement in order to maximize production of ammonia.

Engineers would want to consider several different equilibrium-related factors:

- Temperature—engineers would need to determine the optimal temperature conditions for running the reaction. Since the reaction is exothermic, increasing temperatures shift the reaction towards the reactants.
- Pressure—engineers would consider the fact that increased pressure would shift the reaction to the product, which is desired.
- Concentration—engineers would consider the possibility of removing ammonia (NH3) from the reaction chamber to allow the reaction to continuously shift towards the production of ammonia.
- Catalyst—engineers would consider the use of a catalyst to increase the rate of the reaction. Even though the equilibrium would not be affected by the catalyst, the reaction would proceed and reach the equilibrium faster.





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