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Understanding the behavior of gases in chemical systems is fundamental in chemistry, especially when dealing with reactions involving gaseous reactants and products. In this context, considering a 2.0 L container filled with a mixture of 6.0 moles of carbon monoxide (CO) and 6.0 moles of water vapor (H₂O) provides an excellent example to explore concepts such as gas laws, equilibrium, partial pressures, and the influence of temperature. This article offers an in-depth analysis of the properties, calculations, and implications of such a system, aiming to enhance your understanding of gaseous mixtures in chemical reactions.

Understanding the Initial System: Composition and Conditions

1. The Composition of the Gas Mixture

- The container contains:
- 6.0 moles of carbon monoxide (CO)
- 6.0 moles of water vapor (H₂O)
- Total moles of gases:
- $6.0 + 6.0 = 12.0$ moles
- Volume of the container:
- 2.0 liters

This mixture is a typical setup for studying equilibrium reactions involving gases, such as the water-gas shift reaction or other reversible processes.

2. Initial Parameters and Assumptions

- Temperature (assumed for calculations): commonly standard laboratory conditions ($\sim 25^{\circ}\text{C}$ or 298 K)
- Ideal gas behavior: gases are assumed to behave ideally, which simplifies calculations
- Pressure calculations: based on the ideal gas law ($PV = nRT$)

Applying the Ideal Gas Law to Determine Initial

Conditions

1. The Ideal Gas Law

The ideal gas law provides a basis for calculating the pressure exerted by gases in a fixed volume:

- $PV = nRT$

Where:

- P = pressure (atm)

- V = volume (L)

- n = number of moles

- R = ideal gas constant (0.082057 L·atm/mol·K)

- T = temperature (K)

2. Calculating Total Pressure

Given:

- $n = 12.0$ mol

- $V = 2.0$ L

- $T = 298$ K

Calculation:

$$P = (nRT) / V$$

$$P = (12.0 \text{ mol} \times 0.082057 \text{ L}\cdot\text{atm}/\text{mol}\cdot\text{K} \times 298 \text{ K}) / 2.0 \text{ L}$$

Calculating step-by-step:

- $R \times T = 0.082057 \times 298 \approx 24.45$

- $n \times R \times T = 12.0 \times 24.45 \approx 293.4$

- $P = 293.4 / 2.0 \approx 146.7 \text{ atm}$

Result: The initial total pressure of the gas mixture is approximately 146.7 atm.

Partial Pressures and Mole Fractions

1. Mole Fractions

- Mole fraction of CO:

- $X_{\text{CO}} = \text{moles of CO} / \text{total moles} = 6.0 / 12.0 = 0.5$

- Mole fraction of H₂O:

- $X_{\text{H}_2\text{O}} = 6.0 / 12.0 = 0.5$

2. Partial Pressures

Using Dalton's law:

- $P_{\text{CO}} = X_{\text{CO}} \times P_{\text{total}} = 0.5 \times 146.7 \approx 73.4 \text{ atm}$

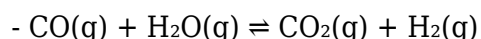
- $P_{\text{H}_2\text{O}} = X_{\text{H}_2\text{O}} \times P_{\text{total}} = 0.5 \times 146.7 \approx 73.4 \text{ atm}$

The equal mole fractions and pressures reflect the symmetric initial conditions of the mixture.

Reactions Involving CO and H₂O in Gaseous Mixtures

1. The Water-Gas Shift Reaction

One of the most common reactions involving CO and H₂O is:



This reaction is important in industrial processes like hydrogen production and in understanding equilibrium in gaseous systems.

2. Equilibrium Considerations

- The reaction is reversible, and its position depends on temperature, pressure, and concentrations.
- At equilibrium, the forward and reverse reaction rates are equal.
- The equilibrium constant (K_{eq}) varies with temperature.

3. Impact of Initial Conditions on Equilibrium

- The initial high pressure (~146.7 atm) favors or disfavors certain reaction directions based on Le Châtelier's principle.
- Changes in temperature can shift the equilibrium position, affecting the composition of the gases.

Calculating Equilibrium Concentrations

1. Equilibrium Expression

For the water-gas shift:

$$K_{\text{eq}} = [\text{CO}_2][\text{H}_2] / [\text{CO}][\text{H}_2\text{O}]$$

Assuming ideal gas behavior:

- Concentrations are proportional to partial pressures:
- $[X] = P_X / RT$

2. Sample Calculation at Equilibrium

Suppose, at a certain temperature, the equilibrium constant K_{eq} is known (say, from literature). To find the equilibrium concentrations:

- Calculate initial partial pressures.

- Establish change variables (e.g., x) to represent the extent of reaction.
- Set up an ICE (Initial, Change, Equilibrium) table.
- Solve for x using the equilibrium expression.

Temperature Effects on Gas Reactions

1. Endothermic vs. Exothermic Reactions

- The water-gas shift can be shifted by temperature:
- Endothermic shift favors the formation of CO and H₂O at higher temperatures.
- Exothermic shifts favor CO₂ and H₂ at lower temperatures.

2. Effect on Partial Pressures and Composition

- Increasing temperature generally decreases the equilibrium constant for exothermic reactions, shifting the equilibrium position.
- Conversely, lowering temperature favors the formation of products.

Practical Implications and Applications

1. Industrial Processes

- The synthesis of hydrogen via the water-gas shift reaction is crucial in fuel cell technology.
- Controlling pressure and temperature allows optimization of product yields.

2. Laboratory Analysis

- Understanding gas mixture behavior aids in designing experiments involving gas reactions.
- Accurate calculations of partial pressures and mole fractions are essential in quantitative analysis.

3. Environmental Considerations

- Managing emissions of CO and H₂O in combustion processes.
- Designing systems to minimize pollution based on understanding gaseous equilibria.

Conclusion

The initial setup of a 2.0 L container charged with 6.0 moles each of CO and H₂O at standard conditions exemplifies fundamental principles of gas laws, chemical equilibrium, and reaction dynamics. By applying the ideal gas law, we calculated the initial total pressure (~146.7 atm) and

partial pressures of each gas. Recognizing the potential for reactions like the water-gas shift, chemists can manipulate temperature and pressure to favor desired products, optimize industrial processes, and understand environmental impacts. Mastery of these concepts enables effective design and analysis of gaseous systems, facilitating advancements across chemical manufacturing, energy production, and environmental management.

Keywords: gas laws, ideal gas law, partial pressure, mole fraction, equilibrium, water-gas shift reaction, CO, H₂O, gas mixture, industrial chemistry

Frequently Asked Questions

What is the total initial pressure inside the 2.0 L container with 6.0 moles of CO and 6.0 moles of H₂O gases?

Using the ideal gas law $PV = nRT$, the total moles are 12.0 mol. Assuming standard temperature (around 298 K) and $R = 0.0821 \text{ L}\cdot\text{atm}/(\text{mol}\cdot\text{K})$, the total pressure is approximately $P = (nRT)/V = (12.0 \times 0.0821 \times 298)/2.0 \approx 146.8 \text{ atm}$.

How does the initial mole ratio of CO to H₂O affect potential chemical reactions in the container?

The initial mole ratio of 1:1 favors reactions where CO and H₂O interact, such as the water-gas shift reaction, and determines the equilibrium position based on reaction stoichiometry and conditions.

What is the significance of the container's volume being 2.0 L for the behavior of the gases?

The small, fixed volume ensures that pressure, concentration, and reaction rates are sensitive to temperature and mole quantities, influencing equilibrium and gas behavior significantly.

What happens to the pressure if the temperature inside the container increases?

An increase in temperature raises the kinetic energy of the gases, leading to an increase in pressure according to Gay-Lussac's law, assuming the amount of gas remains constant.

Can the gases inside the container react with each other, and what conditions favor such reactions?

Yes, CO and H₂O can react via the water-gas shift reaction, especially at elevated temperatures and in the presence of catalysts, shifting equilibrium toward CO₂ and H₂ formation.

How would adding more water vapor influence the equilibrium

of reactions involving CO and H₂O?

Adding more H₂O shifts the equilibrium towards the production of H₂ and CO₂ if the reaction is favorable, according to Le Châtelier's principle.

What are the potential safety considerations for handling such a high-pressure mixture of gases in a small container?

High-pressure gases pose risks of container rupture and explosion. Proper pressure ratings, safety valves, and controlled temperatures are essential to prevent accidents.

How does the mole quantity relate to partial pressures of CO and H₂O in the container?

Partial pressure of each gas is proportional to its mole fraction multiplied by the total pressure. With equal moles, CO and H₂O initially have equal partial pressures if total pressure is known.

What experimental methods can be used to analyze the composition of gases in such a container?

Techniques like gas chromatography, mass spectrometry, or infrared spectroscopy can be used to determine the composition and concentrations of gases inside the container.

How does the initial amount of gases influence the rate of any potential reactions occurring inside the container?

Higher initial quantities of reactants increase the concentration, which can lead to higher reaction rates according to collision theory, especially in the presence of catalysts or elevated temperatures.

Additional Resources

Chemical Equilibrium in a 2.0 L Container: An Expert Analysis of the Mixture of CO(g) and H₂O(g)

Introduction

When exploring the fascinating realm of chemical reactions and equilibria, understanding the behavior of gases in confined spaces becomes paramount. In this detailed review, we examine a scenario involving a 2.0-liter container charged with a mixture of carbon monoxide (CO) and water vapor (H₂O). Specifically, the mixture contains 6.0 moles of each gas, presenting an intriguing case for analyzing chemical equilibrium, reaction dynamics, and the influence of various factors.

This analysis is crucial for chemists, chemical engineers, and students alike, as it encapsulates core concepts of gas behavior, reaction kinetics, and thermodynamics within a manageable, real-world context.

The System: Composition and Initial Conditions

Composition Details

- Container Volume: 2.0 L
- Moles of CO: 6.0 mol
- Moles of H₂O: 6.0 mol

This initial state sets the stage for potential reactions, particularly focusing on the well-known water-gas shift equilibrium:



Significance of the System

This reaction is vital in industrial processes such as hydrogen production and syngas purification. Analyzing the initial conditions helps in understanding how the system evolves towards equilibrium and what factors influence the position of equilibrium.

Fundamental Concepts Explored

Gas Behavior under Ideal Conditions

In this scenario, gases are assumed to behave ideally, which simplifies the calculation of partial pressures and equilibrium constants. Ideal gas law:

$$PV = nRT$$

where:

- P = pressure
- V = volume (2.0 L)
- n = number of moles
- R = ideal gas constant (0.08206 L·atm/(mol·K))
- T = temperature (assumed constant unless specified)

Calculating Initial Partial Pressures

Using the ideal gas law, the initial partial pressures of CO and H₂O are:

$$P = \frac{nRT}{V}$$

Assuming a temperature of 298 K (room temperature):

$$P_{\mathrm{CO}} = \frac{6.0 \times 0.08206 \times 298}{2.0} \approx 73.2, \text{ atm}$$

$$P_{\text{H}_2\text{O}} = \frac{6.0 \times 0.08206 \times 298}{2.0} \approx 73.2 \text{ atm}$$

Thus, both gases initially exert substantial partial pressures, setting significant potential for reaction progression.

The Water-Gas Shift Reaction: Dynamics and Equilibrium

Reaction Overview

The water-gas shift:



is a reversible process where the system may shift to the right or left depending on conditions like temperature, pressure, and initial concentrations.

Equilibrium Constant (K)

The equilibrium constant, K_{eq} , for this reaction at a given temperature, defines the ratio of product activities to reactant activities:

$$K_{\text{eq}} = \frac{P_{\text{CO}_2} \times P_{\text{H}_2}}{P_{\text{CO}} \times P_{\text{H}_2\text{O}}}$$

At standard conditions ($\sim 25^\circ\text{C}$), K_{eq} is approximately 0.5, but it varies significantly with temperature.

Factors Affecting the Equilibrium

1. **Temperature:** The reaction is exothermic ($\sim -41 \text{ kJ/mol}$). Increasing temperature shifts equilibrium toward reactants, decreasing K_{eq} .
2. **Pressure:** As a gaseous reaction with equal molar quantities of reactants and products, pressure changes have minimal impact on the equilibrium position, per Le Chatelier's principle.
3. **Initial Concentrations:** The initial moles influence the reaction pathway, but the system ultimately reaches a state dictated by thermodynamic parameters.

Calculating Equilibrium Composition

Establishing an ICE Table

Let's define:

- x): moles of CO and H₂O reacted at equilibrium

Initial moles:

Species	Initial (mol)	Change (mol)	Equilibrium (mol)
CO	6.0	-x	6.0 - x
H ₂ O	6.0	-x	6.0 - x
CO ₂	0	+x	x
H ₂	0	+x	x

Partial pressures at equilibrium:

$$P_i = \frac{n_i RT}{V}$$

which simplifies calculations based on moles.

Expression for K_{eq}

$$K_{eq} = \frac{(x \times RT/V) \times (x \times RT/V)}{(6.0 - x) \times RT/V \times (6.0 - x) \times RT/V}$$

Since (RT/V) appears in numerator and denominator, it cancels out, yielding:

$$K_{eq} = \frac{x^2}{(6.0 - x)^2}$$

Thus,

$$\sqrt{K_{eq}} = \frac{x}{6.0 - x}$$

Given the K_{eq} value (say, 0.5):

$$\sqrt{0.5} \approx 0.7071 = \frac{x}{6.0 - x}$$

Solving for x :

$$x = 0.7071(6.0 - x)$$

$$x = 4.2426 - 0.7071x$$

\]

\[

$$x + 0.7071x = 4.2426$$

\]

\[

$$1.7071x = 4.2426$$

\]

\[

$$x \approx 2.486, \text{ mol}$$

\]

Final Equilibrium Moles

Species	Moles at Equilibrium
CO	$6.0 - 2.486 \approx 3.514 \text{ mol}$
H ₂ O	3.514 mol
CO ₂	2.486 mol
H ₂	2.486 mol

Final Partial Pressures

Using the ideal gas law:

\[

$$P_i = \frac{n_i RT}{V}$$

\]

with (n_i) as above, (T) at 298 K:

\[

$$P_i \approx \frac{n_i \times 0.08206 \times 298}{2.0} \approx n_i \times 12.2, \text{ atm}$$

\]

Thus,

$$- (P_{\text{CO}} \approx 3.514 \times 12.2 \approx 42.8, \text{ atm})$$

$$- (P_{\text{H}_2\text{O}} \approx 42.8, \text{ atm})$$

$$- (P_{\text{CO}_2} \approx 2.486 \times 12.2 \approx 30.3, \text{ atm})$$

$$- (P_{\text{H}_2} \approx 30.3, \text{ atm})$$

Practical Implications and Applications

Industrial Significance

Understanding the equilibrium behavior of this system is vital in industries where hydrogen production and CO management are critical. The reaction's sensitivity to temperature allows engineers to optimize conditions for desired product yields.

Effect of Temperature Variations

- Higher Temperatures: Favor the reactants (CO and H₂O), reducing hydrogen and CO₂ yields.
- Lower Temperatures: Shift equilibrium toward products, increasing H₂ and CO₂ concentrations.

Real-World Considerations

While calculations assume ideality and constant temperature, real systems involve:

- Catalysts (e.g., iron or copper-based), accelerating reaction rates.
- Non-ideal gas behavior at high pressures.
- Dynamic temperature and pressure conditions.

Potential for Further Optimization

- Adjusting temperature and pressure based on desired outputs.
- Using catalysts to lower activation energy and speed up equilibrium attainment.
- Monitoring gas compositions via spectroscopy or chromatography for process control.

Conclusion

The analysis of a 2.0 L container charged with equal moles of CO and H₂O reveals the intricate balance of chemical reactions under constrained conditions. The water-gas shift reaction exemplifies how initial concentrations, thermodynamic parameters, and external conditions shape the equilibrium state.

Through detailed calculations and understanding of fundamental principles, engineers and chemists can predict system behavior, optimize industrial processes, and innovate more efficient methods for gas management. This scenario encapsulates core chemical concepts, from ideal gas laws to equilibrium dynamics, illustrating the rich complexity underlying seemingly simple gas mixtures.

Final Thoughts

Grasping the nuances of such systems not only enhances theoretical knowledge but also empowers practical applications in energy production, environmental management, and chemical manufacturing. The behavior of gases in a confined environment remains a cornerstone of chemical science, offering endless avenues for exploration and innovation.

Note: Actual equilibrium constants and reaction conditions vary with temperature and pressure. For precise modeling, refer to thermodynamic data specific to the operating conditions.

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