To calculate an equilibrium concentration from an equilibrium constant, an understanding of the concept of equilibrium and how to write an equilibrium constant is required. Equilibrium is a state of dynamic balance where the ratio of the product and reactant concentrations is constant.

Introduction

An equilibrium constant, $K_c$, is the ratio of the concentrations of the products to the concentrations of the reactants at equilibrium. The concentration of each species is raised to the power of that species' coefficient in the balanced chemical equation. For example, for the following chemical equation,

\[
aA + bB \rightleftharpoons cC + dD
\]

the equilibrium constant is written as follows:

\[
K_c = \dfrac{[C]^c [D]^d}{[A]^a [B]^b}
\]

The ICE Table

The easiest approach for calculating equilibrium concentrations is to use an ICE Table, which is an organized method to track which quantities are known and which need to be calculated. ICE stands for:

- "I" is for the "initial" concentration or the initial amount
- "C" is for the "change" in concentration or change in the amount from the initial state to equilibrium
- "E" is for the "equilibrium" concentration or amount and represents the expression for the amounts at equilibrium.

Example 1: Hydrogenation of Ethylene ($C_2H_4$)

For the gaseous hydrogenation reaction below, what is the concentration for each substance at equilibrium?

\[
C_2H_4(g) + H_2(g) \rightleftharpoons C_2H_6(g)
\]

with $K_c = 0.98$ characterized from previous experiments and with the following initial concentrations:

- $[C_2H_4]_0 = 0.33$
- $[H_2]_0 = 0.53$

SOLUTION

First the equilibrium expression is written for this reaction:

\[
K_c = \dfrac{[C_2H_6]}{[C_2H_4][H_2]} = 0.98
\]

ICE Table
The concentrations for the reactants are added to the "Initial" row of the table. The initial amount of \((\text{C}_2\text{H}_6)\) is not mentioned, so it is given a value of 0. This amount will change over the course of the reaction.

<table>
<thead>
<tr>
<th>ICE</th>
<th>((\text{C}_2\text{H}_4))</th>
<th>((\text{H}_2))</th>
<th>((\text{C}_2\text{H}_6))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>0.33</td>
<td>0.53</td>
<td>0</td>
</tr>
<tr>
<td>Change</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Equilibrium</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The change in the concentrations are added to the table. Because ethane, \(\text{C}_2\text{H}_6\) is a product, and there cannot have negative concentrations, the reactants must decrease in stoichiometric intervals. To represent this, a positive or negative "x" is added to each column in the ICE table—reactant concentrations change by -x, and product concentrations change by +x.

<table>
<thead>
<tr>
<th>ICE</th>
<th>((\text{C}_2\text{H}_4))</th>
<th>((\text{H}_2))</th>
<th>((\text{C}_2\text{H}_6))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>0.33</td>
<td>0.53</td>
<td>0</td>
</tr>
<tr>
<td>Change</td>
<td>-x</td>
<td>-x</td>
<td>+x</td>
</tr>
<tr>
<td>Equilibrium</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Equilibrium is determined by adding "Initial" and "Change together.

<table>
<thead>
<tr>
<th>ICE</th>
<th>((\text{C}_2\text{H}_4))</th>
<th>((\text{H}_2))</th>
<th>((\text{C}_2\text{H}_6))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>0.33</td>
<td>0.53</td>
<td>0</td>
</tr>
<tr>
<td>Change</td>
<td>-x</td>
<td>-x</td>
<td>+x</td>
</tr>
<tr>
<td>Equilibrium</td>
<td>0.33-x</td>
<td>0.53-x</td>
<td>x</td>
</tr>
</tbody>
</table>

The expressions in the "Equilibrium" row are substituted into the equilibrium constant expression to find calculate the value of x. The equilibrium expression is simplified into a quadratic expression as shown:

\[
0.98 = \frac{x}{(0.33-x)(0.53-x)}
\]

\[
0.98 = \frac{x^2 - 0.86x + 0.1749}{(x^2 - 0.86x + 0.1749)}
\]
\[0.98 \{x^2 - 0.86x + 0.1749\} = x\]  
\[0.98x^2 - 0.8428x + 0.171402 = x\]  
\[0.98x^2 - 1.8428x + 0.171402 = 0\]

The quadratic formula can be used as follows to solve for x:

\[x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}\]

\[x = \frac{-0.1572 \pm \sqrt{(-0.1572)^2 - 4(0.98)(0.171402)}}{2(0.98)}\]

\[x = 1.78\text{ or } 0.098\]

Because there are two possible solutions, each must be checked to determine which is the real solution. They are plugged into the expression in the "Equilibrium" row for \([C_{2}H_{4}]_{Eq}\):

\([C_{2}H_{4}]_{Eq} = (0.33-1.78) = -1.45\]

\([C_{2}H_{4}]_{Eq} = (0.33-0.098) = 0.23\]

If \(x = 1.78\) then \([C_{2}H_{4}]_{Eq}\) is negative, which is impossible, therefore, \(x\) must equal 0.098.

So:

\([C_{2}H_{4}]_{Eq} = 0.23\text{ M}\]

\([H_{2}]_{Eq} = (0.53-0.0981) = 0.43\text{ M}\]

\([C_{2}H_{6}]_{Eq} = 0.098\text{ M}\]

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### Problems

1. Find the concentration of iodine in the following reaction if the equilibrium constant is \(3.76 \times 10^3\), and 2 mol of iodine are initially placed in a 2 L flask at 100 K.

\(I_{2(g)} \rightleftharpoons 2I^-_{(aq)}\)

2. What is the concentration of silver ions in 1.00 L of solution with 0.020 mol of AgCl and 0.020 mol of Cl\(^-\) in the following reaction? The equilibrium constant is \(1.8 \times 10^{-10}\).

\(AgCl_{(s)} \rightleftharpoons Ag^{+}_{(aq)} + Cl^{-}_{(aq)}\)

3. What are the equilibrium concentrations of the products and reactants for the following equilibrium reaction?
Initial concentrations: \([\text{HSO}_4^-]_0 = 0.4 \) \([\text{H}_3\text{O}^+]_0 = 0.01\) \([\text{SO}_4^{2-}]_0= 0.07\) \(K=.012\)

\[\text{HSO}_4^-(aq) + \text{H}_2\text{O}(l) \rightleftharpoons \text{H}_3\text{O}^+(aq) + \text{SO}_4^{2-}(aq) \]

4. The initial concentration of HCO\(_3\) is 0.16 M in the following reaction. What is the \(H^+\) concentration at equilibrium? \(K_c=0.20\).

\[\text{H}_2\text{CO}_3 \rightleftharpoons \text{H}^+(aq) + \text{CO}_3^{2-}(aq)\]

5. The initial concentration of PCl\(_5\) is 0.200 moles per liter and there are no products in the system when the reaction starts. If the equilibrium constant is 0.030, calculate all the concentrations at equilibrium.

**Solutions**

1.

<table>
<thead>
<tr>
<th></th>
<th>([I_2])</th>
<th>([I^-])</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Initial</strong></td>
<td>2mol/2L = 1 M</td>
<td>0</td>
</tr>
<tr>
<td><strong>Change</strong></td>
<td>(-x)</td>
<td>(+2x)</td>
</tr>
<tr>
<td><strong>Equilibrium</strong></td>
<td>(1-x)</td>
<td>(2x)</td>
</tr>
</tbody>
</table>

At equilibrium

\[(K_c=\dfrac{[I^-]^2}{[I_2]})\]

\[3.76 \times 10^3=\dfrac{(2x)^2}{1-x} = \dfrac{4x^2}{1-x}\]

cross multiply

\[(4x^2+3.76 \times 10^3x-3.76 \times 10^3=0)\]

apply the quadratic formula:

\[\left( \dfrac{-b \pm \sqrt{b^2 - 4ac}}{2a} \right)\]

with: \((a=4)\), \((b=3.76 \times 10^3)\), \((c=-3.76 \times 10^3)\).

The formula gives solutions of x=0.999 and -940. The latter solution is unphysical (a negative concentration). Therefore, \(x=0.999\) at equilibrium.

\([I^-]=2x=1.99 \) M

\([I_2]=1-x=1-.999=0.001\) M
2. 

<table>
<thead>
<tr>
<th></th>
<th>((\text{Ag}^+}))</th>
<th>((\text{Cl}^-}))</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Initial</strong></td>
<td>0</td>
<td>0.02 mol/1.00 L = 0.02 M</td>
</tr>
<tr>
<td><strong>Change</strong></td>
<td>((-x))</td>
<td>((+x))</td>
</tr>
<tr>
<td><strong>Equilibrium</strong></td>
<td>((x))</td>
<td>((0.02 + x))</td>
</tr>
</tbody>
</table>

\[ K_c = [\text{Ag}^+] [\text{Cl}^-] \]

\[ 1.8 \times 10^{-10} = (x)(0.02 + x) \]

\[ x^2 + 0.02x - 1.8 \times 10^{10} = 0 \]

\[ x = 9 \times 10^{-9} \]

\[ [\text{Ag}^+] = 9 \times 10^{-9} \]

\[ [\text{Cl}^-] = 0.02 + x = 0.020 \]

3. 

<table>
<thead>
<tr>
<th></th>
<th>((\text{H}_2\text{CO}_3}))</th>
<th>((\text{SO}_4^{2-}}))</th>
<th>((\text{H}_3\text{O}^+}))</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Initial</strong></td>
<td>0.4</td>
<td>0.01</td>
<td>0.07</td>
</tr>
<tr>
<td><strong>Change</strong></td>
<td>((-x))</td>
<td>((+x))</td>
<td>((+x))</td>
</tr>
<tr>
<td><strong>Equilibrium</strong></td>
<td>((0.4-x))</td>
<td>((0.01+x))</td>
<td>((0.07+x))</td>
</tr>
</tbody>
</table>

\[ K_c = \left(\text{SO}_4^{2-}\right) \left(\text{H}_3\text{O}^+\right) / \left(\text{H}_2\text{CO}_3\right) \]

\[ 0.012 = \left(0.01 + x\right) \left(0.07 + x\right) / (0.4 - x) \]

cross multiply and get:

\[ x^2 + 0.2x - 0.0041 = 0 \]

apply the quadratic formula

\[ x = 0.0328 \]

\[ [\text{H}_2\text{CO}_3] = 0.4 - x = 0.4 - 0.0328 = 0.3672 \]

\[ [\text{SO}_4^{2-}] = 0.01 + x = 0.01 + 0.0328 = 0.0428 \]
4. 

\[
[H_3O]^+ = 0.07 + x = 0.07 + 0.0328 = 0.1028
\]

<table>
<thead>
<tr>
<th></th>
<th>(H_2CO_3)</th>
<th>((H^+)^+)</th>
<th>((CO_3^{2-})^{2-})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>0.16</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Change</td>
<td>-x</td>
<td>+x</td>
<td>+x</td>
</tr>
<tr>
<td>Equilibrium</td>
<td>0.16-x</td>
<td>x</td>
<td>x</td>
</tr>
</tbody>
</table>

\[
K_c = [CO_3^{2-}][H^+]/[H_2CO_3]
\]

apply the quadratic equation

\[
x = 0.1049
\]

\[
[H^+]=x=0.1049
\]

5. First write out the balanced equation:

\[
PACL_5(g) \rightleftharpoons PCl_3(g) + Cl_2(g)
\]

<table>
<thead>
<tr>
<th></th>
<th>(PCl_5)</th>
<th>(PCl_3)</th>
<th>(Cl_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>0.2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Change</td>
<td>-x</td>
<td>+x</td>
<td>+x</td>
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<tr>
<td>Equilibrium</td>
<td>0.2-x</td>
<td>x</td>
<td>x</td>
</tr>
</tbody>
</table>

\[
K_c = \dfrac{[PCl_3][Cl_2]}{[PCl_5]}\]

\[
0.30 = \dfrac{x^2}{0.2-x}\]

Cross multiply:

\[
x^2 + 0.03 x - 0.006 = 0
\]

Apply the quadratic formula:

\[
x = 0.064
\]

\[
[PCl_5]=0.2-x=0.136
\]

\[
[PCl_3]=0.064
\]
[Cl₂]=0.064

References


Contributors