Reaction Quotient

How do you predict which direction a reaction will proceed to reach equilibrium?

**Why?**

When a reaction reaches equilibrium there must be some non-negligible amount of every species in the reaction, otherwise the reaction cannot react in both directions. Knowing this, it is very easy to predict which direction a reaction will go to reach equilibrium when one of the components of the reaction has an initial concentration of zero. Many of the problems you have worked with thus far have some component at zero concentration, but real life does not work that way. Most of the time, the reaction in question has some measurable amount of every species. Deciding which way the reaction will go to reach equilibrium then becomes more challenging.

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**Model 1 – A Theoretical Equilibrium**

<table>
<thead>
<tr>
<th>Trial 1</th>
<th>A(g) + B(g) ⇌ C(g)</th>
<th>Trial 2</th>
<th>A(g) + B(g) ⇌ C(g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>1.000 M</td>
<td>1.000 M</td>
<td>1.000 M</td>
</tr>
<tr>
<td>Change</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Equilibrium</td>
<td>1.464 M</td>
<td>1.464 M</td>
<td>0.536 M</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Trial 3</th>
<th>A(g) + B(g) ⇌ C(g)</th>
<th>Trial 4</th>
<th>A(g) + B(g) ⇌ C(g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>1.000 M</td>
<td>0.500 M</td>
<td>1.500 M</td>
</tr>
<tr>
<td>Change</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Equilibrium</td>
<td>1.864 M</td>
<td>1.364 M</td>
<td>0.636 M</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Trial 5</th>
<th>A(g) + B(g) ⇌ C(g)</th>
<th>Trial 6</th>
<th>A(g) + B(g) ⇌ C(g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>1.400 M</td>
<td>1.200 M</td>
<td>0.400 M</td>
</tr>
<tr>
<td>Change</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Equilibrium</td>
<td>1.388 M</td>
<td>1.188 M</td>
<td>0.412 M</td>
</tr>
</tbody>
</table>

1. Examine Model 1.
   
   a. Write the theoretical chemical reaction that is used in the trials of Model 1.
   
   b. If 0.50 M of reactant A reacts, predict the change in concentration of B and C.

2. What variables were changed in the different trials shown in Model 1?
3. In Trial 1 of Model 1 there is an arrow in the “change” section of the table.
   a. Explain what that arrow represents.

   b. What evidence is present in the table to indicate the direction the arrow should be pointing?

4. With your group, determine which direction each of the other trials in Model 1 reacted to reach equilibrium. Indicate that direction with an arrow in the “change” section of the table.

5. Is it true that there are equal concentrations of reactants and products when all of the reactions in Model 1 reach equilibrium? Justify your answer with evidence from Model 1.

6. According to Model 1, are the final concentrations of all species in the reaction the same when the reaction reaches equilibrium, regardless of the initial concentration?

7. Does the reaction in Model 1 always proceed in the forward direction when there are more reactants than products? Justify your answer with evidence from Model 1.

8. Write the equilibrium constant expression for the reaction in Model 1.

9. Discuss with your group how you could determine the equilibrium constant, \( K_{eq} \), for the reaction in Model 1. Divide the work among group members. Use data from multiple trials to calculate the equilibrium constant for the reaction and determine the average. Show all work.
Read This!
The key to knowing which direction a reaction will need to proceed in order to reach equilibrium is knowing if you have too much reactant or too much product compared to the equilibrium state. Keep in mind, however, that there are many combinations of reactant and product concentrations that constitute an equilibrium state.

Model 2 – Comparing \(Q\) and \(K_{\text{eq}}\)

<table>
<thead>
<tr>
<th>Trial</th>
<th>Reaction Quotient, (Q)</th>
<th>Equilibrium Constant, (K_{\text{eq}})</th>
<th>(Q) versus (K_{\text{eq}})</th>
<th>Direction to Equilibrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
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<tr>
<td>6</td>
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</tr>
</tbody>
</table>

10. Fill in the Equilibrium Constant column in Model 2 using data from Model 1.
11. Fill in the Direction to Equilibrium column in Model 2 using data from Model 1.

Read This!
The reaction quotient for a reaction is the ratio of products to reactants, similar to the equilibrium constant. The difference is you calculate the ratio with initial conditions.

\[
K_{\text{eq}} = \frac{[C]_{eq}}{[A]_{eq}[B]_{eq}} \quad Q = \frac{[C]_{\text{initial}}}{[A]_{\text{initial}}[B]_{\text{initial}}}
\]

12. Calculate the reaction quotient for each of the trials in Model 1 and record the data in Model 2 in the appropriate column. Divide the work among group members. Show your work below.
13. Consider how the concentration values in the reaction quotient change when the reaction proceeds in the forward direction.
   a. Does the numerator increase or decrease?

   b. Does the denominator increase or decrease?

   c. Overall, does the $Q$ ratio increase or decrease when the reaction proceeds in the forward direction?

14. Consider how the concentration values in the reaction quotient change when the reaction proceeds in the reverse direction.
   a. Does the numerator increase or decrease?

   b. Does the denominator increase or decrease?

   c. Overall does the $Q$ ratio increase or decrease when the reaction proceeds in the forward direction?

15. Fill in the $Q$ versus $K_{eq}$ column in the table in Model 2. Write $Q > K_{eq}$, $Q < K_{eq}$ or $Q = K_{eq}$.

16. Complete the following statements.
   a. When the reaction quotient is greater than the equilibrium constant, the reaction proceeds more in (the forward, the reverse, neither) direction to reach equilibrium.

   b. When the reaction quotient is less than the equilibrium constant, the reaction proceeds more in (the forward, the reverse, neither) direction to reach equilibrium.

   c. When the reaction quotient is equal to the equilibrium constant, the reaction proceeds more in (the forward, the reverse, neither) direction to reach equilibrium.
17. Consider the following reaction.  
\[ 2\text{SO}_2 \text{(g)} + \text{O}_2 \text{(g)} \leftrightharpoons 2\text{SO}_3 \text{(g)} \]  
\[ K_{eq} = 3900 \text{ at } 2000 \text{ K} \]

a. Write the equilibrium constant expression for the reaction.

b. Write the reaction quotient expression for the reaction.

c. A reaction vessel contains 0.150 M sulfur dioxide, 0.150 M oxygen and 2.000 M sulfur trioxide. Predict the direction the reaction must shift to reach equilibrium. Show a calculation to justify your answer.

18. Consider the following reaction.  
\[ 2\text{HI} \text{(g)} \leftrightharpoons \text{H}_2 \text{(g)} + \text{I}_2 \text{(g)} \]  
\[ K_{eq} = 0.25 \text{ at } 25 \, ^\circ\text{C} \]

A reaction vessel contains 0.500 M hydrogen, 0.500 M iodine vapor and 0.750 M hydrogen iodide. Predict the direction the reaction must shift to reach equilibrium. Show a calculation to justify your answer.
Extension Questions

19. Consider the following reaction.

\[ \text{Cd}^{2+}(aq) + 4\text{Cl}^- (aq) \rightleftharpoons \text{CdCl}_4^{2-} (aq) \quad K_{eq} = 108 \text{ at } 25 \, ^\circ \text{C} \]

a. Write the reaction quotient expression for the reaction.

b. A reaction vessel contains 0.100 M cadmium ion, 0.500 M chloride and 0.250 M tetrachlororcadmate ion. Predict the direction the reaction must shift to reach equilibrium. Show a calculation to justify your answer.

20. Consider the following reaction.

\[ \text{C} (s) + \text{H}_2\text{O} (g) \rightleftharpoons \text{H}_2 (g) + \text{CO} (g) \quad K_{eq} = 4.09 \times 10^{-3} \text{ at } 2000 \, ^\circ \text{K} \]

a. A 1.000-L reaction vessel contains 4.00 M of water vapor, 0.040 M hydrogen and 0.040 M carbon monoxide. Calculate the reaction quotient and state which direction the quotient predicts the reaction must shift to reach equilibrium.

b. Discuss why the prediction above is wrong in this case.

21. LeChâtelier’s principle states that an equilibrium system will shift in the direction that reduces the stress put on the system. Is this consistent with the predictions made by calculating the reaction quotient and comparing \( Q \) to the equilibrium constant? Provide an example to support your answer.