Answer Key: Q, K, and Le Chatelier Part 1

Pre-Activity Questions

1. Describe equilibrium from a macroscopic and microscopic point of view.
   Macro – the reaction exhibits no further observable change
   Micro – the rate of the forward reaction equals the rate of the reverse reaction therefore the concentrations of all species are constant

   Especially if doing as a review activity, might be good to discuss that equilibrium is a concept that applies to reversible reactions and maybe use an example like weak acids versus strong acids or dissolving of salts (in that if it has not exceeded solubility it is not at equilibrium). Those examples in particular might be helpful for the Day 2 demo.

2. State Le Chatelier’s principle.
   EK6.B.1 – Systems at equilibrium respond to disturbances by partially countering the effect of the disturbance.
   Might be useful to review general stresses and responses like adding/removing species, changes in volume/pressure of gaseous species, and dilution of an aqueous system with water as the solvent (though could more broadly be any system and its solvent).
   Would be helpful to note that Le Chatelier’s only applies to a system at equilibrium so you would not use it to qualitatively discuss which direction a reaction will proceed from initial conditions.

3. What is Q? What does it mean if Q is greater than K? What does it mean if Q is less than K?
   Q is the same as K, but the concentrations/pressures can be at any given point versus only at equilibrium for K. I explain to my students that both Q/K is essentially a ratio of product over reactant. So then if Q is too big, there is too much product, therefore product will be consumed, reactant will be produced, and the reaction will shift left to reach equilibrium. If Q is too small, there is too much reactant, therefore reactant will be consumed, product will be produced, and the reaction will shift right to reach equilibrium. Q vs K is always an acceptable qualitative comparison when the concentration of a species changes. It is the only acceptable comparison given initial conditions for consideration.

Activity Questions

Data Table

<table>
<thead>
<tr>
<th></th>
<th>Initial</th>
<th>Equilibrium</th>
<th>New Initial</th>
<th>New Equilibrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>[A]</td>
<td>0.800 M</td>
<td>0.355 M</td>
<td>0.355 M</td>
<td>0.172 M</td>
</tr>
<tr>
<td>[B]</td>
<td>0.600 M</td>
<td>0.155 M</td>
<td>0.800 M</td>
<td>0.617 M</td>
</tr>
<tr>
<td>[C]</td>
<td>0.050 M</td>
<td>0.495 M</td>
<td>0.495 M</td>
<td>0.678 M</td>
</tr>
<tr>
<td>[D]</td>
<td>0.000 M</td>
<td>0.445 M</td>
<td>0.445 M</td>
<td>0.628 M</td>
</tr>
</tbody>
</table>

4. Go to the website listed below. It will open an equilibrium simulation.
   http://employees.oneonta.edu/viningwj/sims/disturbing_a_chemical_equilibrium_s.html
5. Write the reaction, equilibrium expression, and K value.

\[ A + B \rightleftharpoons C + D \]

\[ K = \frac{[C][D]}{[A][B]} = 4.0 \]

a. What does the magnitude of K indicate about the reaction mixture at equilibrium?
Since K is greater than 1, there is more product (C, D) at equilibrium than reactant (A, B).

b. What does the value of K indicate about the rate constant of the forward reaction compared to the rate constant of the reverse reaction?
Rate constant of the forward reaction is four times greater than the rate constant of the reverse reaction favoring the formation of product.

c. Calculate the value of \( \Delta G^\circ \) for the reaction. What does the sign and magnitude of \( \Delta G^\circ \) indicate about the reaction?
-3.4 kJ/mol, small negative means it is thermodynamically favorable, the system is capable of doing work, but not very much.

6. Record the initial concentrations of the species A, B, C, and D in the Data Table.

7. Click the equilibrate button.
   a. Looking at the graph, what point on the graph indicates that equilibrium has been reached? Explain.
   On the x-axis, when all the curves plateau. The plateau indicates that the concentration is no longer changing (thinking about rates, it is where the instantaneous rate for all the species is the same).

   b. Briefly compare and contrast how the concentrations of A, B, C, and D changed during the course of the reaction.
The products both gain 0.445M and the reactants each lose 0.445M.

8. Increase the concentration of species B to 0.800 M. Record the new initial concentrations of all the species in the Data Table.

9. Click the equilibrate button.
   a. Record the new equilibrium concentrations in the Data Table.
   b. How does the graph illustrate the sudden increase in the concentration of species B?
The time is marked with the dashed line starting from the x-axis and there is a huge spike in the black line corresponding to the sudden injection of more B to the reaction.

   c. Looking at the graph, what point on the graph indicates that equilibrium has been reached? Explain.
   Same as before – plateaus

   d. Briefly compare and contrast how the concentrations of A, B, C, and D changed from the new initial to the end of the reaction.
Both A and B are consumed by 0.183M and both C and D are produced by 0.183M. If using as review, might be good to stop and point out that these numbers are simple because all the mole ratios are 1.
e. Explain the change from “new initial” to “new equilibrium” using Le Chatelier’s principle.
The addition of B to the system requires the reaction to consume the added B, which leads to the consumption of A and production of C and D as the system shifts to reestablish equilibrium.

f. Explain the change from “new initial” to “new equilibrium” by comparing Q vs. K.
The addition of B to the system decreases Q since B is a reactant in the denominator, therefore the system will adjust by consuming reactants and producing products until Q equals K.

10. Reset the simulation. Run it a few more times, changing concentrations of the species in different ways. Encourage them to change reactants and products and have them take turns explaining changes within their groups.

Post-Activity Questions

11. Think about the change in concentration from “initial” to “equilibrium.” Would Le Chatelier’s principle or a comparison of Q vs. K be most appropriate to justify that change? Explain your answer.

Q vs K since the system was not disturbed at equilibrium.

12. Consider the reaction shown below. The reaction has a K value of $4 \times 10^{-1}$.

\[ A(g) + B(g) \rightarrow C(g) + D(g) \]

a. At equilibrium, will there be a greater concentration of product, a greater concentration of reactant, or equal concentrations of both? Explain your answer.

More reactant than product since K is less than 1

b. Suppose a 1 L reaction vessel is initially charged with 5 molecules of each species (A, B, C, and D) and then sealed.

i. In the labeled boxes below, depict the number and species of particles present initially and then at equilibrium. Explain your answer.

<table>
<thead>
<tr>
<th>Initial</th>
<th>Equilibrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>A A A A A</td>
<td>A A A A A A A</td>
</tr>
<tr>
<td>B B B B B</td>
<td>B B B B B B B</td>
</tr>
<tr>
<td>C C C C C</td>
<td>C C C</td>
</tr>
<tr>
<td>D D D D D</td>
<td>D D D</td>
</tr>
</tbody>
</table>

Ideally kids would draw them spread around the entire box since they are gases, but there should be five of each representing Q=1, therefore to reach equilibrium, product must be consumed to reach K=0.4.

This distribution leads to Q=0.43 which is as close as we can get with this number of particles. A common misconception is for student diagrams to arbitrarily show more reactant than product without considering the meaning of K.
c. The reaction reaches equilibrium. Consider each of the following stresses and explain how, if at all, the concentrations of A, B, C, and D will change in response to the stress.

   i. Molecules of B are added to the reaction vessel.
   ii. Molecules of D are added to the reaction vessel.
   iii. Molecules of C are removed from the reaction vessel.
   iv. The volume of the reaction vessel is halved.

   i. shift to produce more product
   ii. shift to produce more reactant
   iii. shift to produce more product
   iv. no change since the change does not produce a change in Q

**Note for Teachers:** There is another great equilibrium simulation that neatly illustrates K, k, and Q. The link is below. The simulation requires a little more thinking so it might be a useful homework assignment as part of this activity.
http://glencoe.mheducation.com/olcweb/cgi/pluginpop.cgi?it=swf::800::600::/sites/dl/free/0035715985/117354/Equil_Nav.swf::Equilibrium%20Simulation