Pearson

15.6: Calculating the Equilibrium Constant from Measured Equilibrium Concentrations

The most direct way to obtain an experimental value for the equilibrium constant of a reaction is to measure the concentrations of the reactants and products in a reaction mixture at equilibrium. Consider again the reaction between hydrogen and iodine to form hydrogen iodide:

$$H_2(g) + I_2(g) \rightleftharpoons 2\ HI(g)$$

We saw in Table 15.1 (see Section 15.3) that the measured concentrations of the reactants and products, when substituted into the expression for *K*, always equal a constant (the equilibrium constant) at a constant temperature. For example, one set of measurements at 445 °C results in equilibrium concentrations of $[H_2] = 0.11\ M,\ [I_2] = 0.11\ M$, and $[HI] = 0.78\ M$. What is the value of the equilibrium constant at this temperature? We can write the expression for K_c from the balanced equation and substitute the equilibrium concentrations to obtain the value of K_c:

$$\begin{aligned} K_c &= \frac{[HI]^2}{[H_2][I_2]} \\ &= \frac{(0.78)^2}{(0.11)(0.11)} \\ &= 5.0 \times 10^1 \end{aligned}$$

The concentrations within K_c should always be written in moles per liter (M); however, as noted in Section 15.4, we do not normally include the units when expressing the value of the equilibrium constant, so K_c is unitless.

> Because equilibrium constants depend on temperature, many equilibrium problems state the temperature even though it has no formal part in the calculation.

We just calculated the equilibrium constant from values of the equilibrium concentrations of all the reactants and products. In most cases, however, we need only know the initial concentrations of the reactant(s) and the equilibrium concentration of any *one* reactant or product. We can deduce the other equilibrium concentrations from the stoichiometry of the reaction. For example, consider the simple reaction:

$$A(g) \rightleftharpoons 2\ B(g)$$

Suppose that we have a reaction mixture in which the initial concentration of A is 1.00 M and the initial concentration of B is 0.00 M. When equilibrium is reached, the concentration of A is 0.75 M. Since [A] has changed by −0.25 M, we can deduce (based on the stoichiometry) that [B] must have changed by $2 \times (+0.25\ M)$ or +0.50 M. We summarize the initial conditions, the changes, and the equilibrium conditions in the following table:

	[A]	[B]
Initial	1.00	0.00
Change	−0.25	+2(0.25)
Equilibrium	0.75	0.50

The last row in an ICE table is the sum of the two rows above it.

We refer to this type of table as an ICE table (I = initial, C = change, E = equilibrium). To calculate the equilibrium constant, we use the balanced equation to write an expression for the equilibrium constant and then substitute the equilibrium concentrations from the ICE table:

$$K = \frac{[B]^2}{[A]} = \frac{(0.50)^2}{(0.75)} = 0.33$$

In Examples 15.5 and 15.6, the general procedure for solving these kinds of equilibrium problems is in the left column, and two worked examples exemplifying the procedure are in the center and right columns.

Example 15.5 Finding Equilibrium Constants from Experimental Concentration Measurements

Consider the following reaction:

$$CO(g) + 2\,H_2(g) \rightleftharpoons CH_3OH(g)$$

A reaction mixture at $780^{\circ}C$ initially contains $[CO] = 0.500\ M$ and $[H_2] = 1.00\ M$. At equilibrium, the CO concentration is 0.15 M. What is the value of the equilibrium constant?

PROCEDURE To solve these types of problems, follow the given procedure.

1. **Using the balanced equation as a guide, prepare an ICE table showing the known initial concentrations and equilibrium concentrations of the reactants and products.** Leave space in the middle of the table for determining the changes in concentration that occur during the reaction. If initial concentrations of some reactants or products are not given, you may assume they are zero.

$$CO(g) + 2\,H_2(g) \rightleftharpoons CH_3OH(g)$$

	[CO]	$[H_2]$	$[CH_3OH]$
Initial	0.500	1.00	0.00
Change			
Equil	0.15		

2. **For the reactant or product whose concentration is known both initially and at equilibrium, calculate the change in concentration that occurs.**

$$CO(g) + 2\,H_2(g) \rightleftharpoons CH_3OH(g)$$

	[CO]	$[H_2]$	$[CH_3OH]$
Initial	0.500	1.00	0.00
Change	−0.35		
Equil	0.15		

3. **Use the change calculated in Step 2 and the stoichiometric relationships from the balanced chemical equation to determine the changes in concentration of all other reactants and products.** Since reactants are consumed during the reaction, the changes in their concentrations are negative. Since products are formed, the changes in their concentrations are positive.

$$CO(g) + 2\,H_2(g) \rightleftharpoons CH_3OH(g)$$

	[CO]	$[H_2]$	$[CH_3OH]$
Initial	0.500	1.00	0.00
Change	−0.35	−2(0.35)	+0.35
Equil	0.15		

4. Sum each column for each reactant and product to determine the equilibrium concentrations.

	[CO]	[H_2]	[CH_3OH]
Initial	0.500	1.00	0.00
Change	−0.35	−0.70	+0.35
Equil	0.15	0.30	0.35

5. Use the balanced equation to write an expression for the equilibrium constant and substitute the equilibrium concentrations to calculate *K*.

$$\begin{aligned} K_c &= \frac{[CH_3OH]}{[CO]\,[H_2]^2} \\ &= \frac{0.35}{(0.15)\,(0.30)^2} \\ &= 26 \end{aligned}$$

FOR PRACTICE 15.5 The reaction in Example 15.5 between CO and H_2 is carried out at a different temperature with initial concentrations of $[CO] = 0.27$ M and $[H_2] = 0.49$ M. At equilibrium, the concentration of CH_3OH is 0.11 M. Find the equilibrium constant at this temperature.

Example 15.6 Finding Equilibrium Constants from Experimental Concentration Measurements

Consider the following reaction:

$$2\ CH_4(g) \rightleftharpoons C_2H_2(g) + 3\ H_2(g)$$

A reaction mixture at 1700°C initially contains $[CH_4] = 0.115$ M. At equilibrium, the mixture contains $[C_2H_2] = 0.035$ M. What is the value of the equilibrium constant?

PROCEDURE To solve these types of problems, follow the given procedure.

1. Using the balanced equation as a guide, prepare an ICE table showing the known initial concentrations and equilibrium concentrations of the reactants and products. Leave space in the middle of the table for determining the changes in concentration that occur during the reaction. If initial concentrations of some reactants or products are not given, you may assume they are zero.

$$2\ CH_4(g) \rightleftharpoons C_2H_2(g) + 3\ H_2(g)$$

	[CH_4]	[C_2H_2]	[H_2]
Initial	0.115	0.00	0.00
Change			
Equil		0.035	

2. For the reactant or product whose concentration is known both initially and at equilibrium, calculate the change in concentration that occurs.

$$2\ CH_4(g) \rightleftharpoons C_2H_2(g) + 3\ H_2(g)$$

	[CH_4]	[C_2H_2]	[H_2]
Initial	0.115	0.00	0.00
Change		+0.035	
Equil		0.035	

3. Use the change calculated in Step 2 and the stoichiometric relationships from the balanced chemical equation to determine the changes in concentration of all other reactants and products. Since reactants are consumed during the reaction, the changes in their concentrations are negative. Since products are formed, the changes in their concentrations are positive.

$$2\,CH_4(g) \rightleftharpoons C_2H_2(g) + 3\,H_2(g)$$

	$[CH_4]$	$[C_2H_2]$	$[H_2]$
Initial	0.115	0.00	0.00
Change	−2(0.035)	+0.035	+3(0.035)
Equil		0.035	

4. Sum each column for each reactant and product to determine the equilibrium concentrations.

	$[CH_4]$	$[C_2H_2]$	$[H_2]$
Initial	0.115	0.00	0.00
Change	−0.070	+0.035	+0.105
Equil	0.045	0.035	0.105

5. Use the balanced equation to write an expression for the equilibrium constant and substitute the equilibrium concentrations to calculate *K*.

$$\begin{aligned} K_c &= \frac{[C_2H_2]\,[H_2]^3}{[CH_4]^2} \\ &= \frac{(0.035)\,(0.105)^3}{(0.045)^2} \\ &= 0.020 \end{aligned}$$

FOR PRACTICE 15.6 The reaction of CH_4 in Example 15.6 is carried out at a different temperature with an initial concentration of $[CH_4] = 0.087$ M. At equilibrium, the concentration of H_2 is 0.012 M. Find the equilibrium constant at this temperature.

Interactive Worked Example 15.5 **Finding Equilibrium Constants from Experimental Concentration Measurements**