

## 6.7: Solving Equilibrium Problems

An ICE (Initial, Change, Equilibrium) table is simple matrix formalism that used to simplify the calculations in reversible equilibrium reactions (e.g., weak acids and weak bases or complex ion formation).

### Introduction

ICE tables are composed of the concentrations of molecules in solution in different stages of a reaction, and are usually used to calculate the  $K$ , or equilibrium constant expression, of a reaction (in some instances,  $K$  may be given, and one or more of the concentrations in the table will be the unknown to be solved for). ICE tables automatically set up and organize the variables and constants needed when calculating the unknown.

ICE is a simple acronym for the titles of the first column of the table.

- **I** stands for **initial** concentration. This row contains the initial concentrations of products and reactants.
- **C** stands for the **change** in concentration. This is the concentration change required for the reaction to reach equilibrium. It is the difference between the equilibrium and initial rows. The concentrations in this row are, unlike the other rows, expressed with either an appropriate positive (+) or negative (-) sign and a variable; this is because this row represents an increase or decrease (or no change) in concentration.
- **E** is for the concentration when the reaction is at **equilibrium**. This is the summation of the initial and change rows. Once this row is completed, its contents can be plugged into the equilibrium constant equation to solve for  $K_c$ .

The procedure for filling out an ICE table is best illustrated through example.

#### ✓ Example 1

Use an ICE table to determine  $K_c$  for the following balanced general reaction:



where the capital letters represent the products and reactants.

- This equation will be placed horizontally above the table, with each product and reactant having a separate column.

**A sample consisting of 0.500 mol of x is placed into a system with a volume of 0.750 liters.**

- This statement implies that there are no initial amounts of Y and Z. For the I row of the Y and Z columns, 0.000 mol will be entered.
- Notice that the initial composition is given in moles. The amounts can either be converted to concentrations before putting them into the ICE table or after the equilibrium amounts have been calculated. This example uses moles for the ICE table, and calculates concentrations later.

**At equilibrium, the amount of sample x is known to be 0.350 mol.**

- For the equilibrium row of X, 0.350 mol will be entered.

Desired Unknown

$$K_c = ?$$

### Solution

The equilibrium constant expression is expressed as products over reactants, each raised to the power of their respective stoichiometric coefficients:

$$K_c = \frac{[\text{Y}]^3 [\text{Z}]^4}{[\text{X}]^2}$$

The equilibrium concentrations of Y and Z are unknown, but they can be calculated using the ICE table.

#### STEP 1: Fill in the given amounts

Reaction:	2X	3Y	4Z

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Initial amounts	0.500 mol	0.000 mol	0.000 mol
Change in amount	?	?	?
Equilibrium amount	0.350 mol	?	?

This is the first step in setting up the ICE table. As mentioned above, the ICE mnemonic is vertical and the equation heads the table horizontally, giving the rows and columns of the table, respectively. The numerical amounts were given. Any amount not directly given is unknown.

### STEP 2: Fill in the amount of change for each compound

Reaction	2X	3Y	4Z
Initial amounts	0.500 mol	0.000 mol	0.000 mol
Change in amount	-0.150 mol	+0.225 mol	+0.300 mol
Equilibrium amounts	0.350 mol	?	?

Notice that the equilibrium in this equation is shifted to the right, meaning that some amount of reactant will be taken away and some amount of product will be added (for the Change row).

The change in amount ( $x$ ) can be calculated using algebra:

$$\text{Equilibrium Amount} = \text{Initial Amount} + \text{Change in Amount}$$

Solving for the Change in the amount of  $2x$  gives:

$$0.350 \text{ mol} - 0.500 \text{ mol} = -0.150 \text{ mol}$$

The change in reactants and the balanced equation of the reaction is known, so the change in products can be calculated. The stoichiometric coefficients indicate that for every 2 mol of  $x$  reacted, 3 mol of  $Y$  and 4 mol of  $Z$  are produced. The relationship is as follows:

$$\text{Change in Product} = - \left( \frac{\text{Stoichiometric Coefficient of Product}}{\text{Stoichiometric Coefficient of Reactant}} \right) (\text{Change in Reactant}) \quad (6.7.1)$$

$$\text{Change in } Y = - \left( \frac{3}{2} \right) (-0.150 \text{ mol}) \quad (6.7.2)$$

$$= +0.225 \text{ mol} \quad (6.7.3)$$

Try obtaining the change in  $Z$  with this method (the answer is already in the ICE table).

### STEP 3: Solve for the equilibrium amounts

Reaction	2X	3Y	4Z
Initial amounts	0.500 mol	0.000 mol	0.000 mol
Change in amounts	-0.150 mol	+0.225 mol	+0.300 mol
Equilibrium amounts	0.350 mol	0.225 mol	0.300 mol

If the initial amounts of  $Y$  and/or  $Z$  were nonzero, then they would be added together with the change in amounts to determine equilibrium amounts. However, because there was no initial amount for the two products, the equilibrium amount is simply equal to the change:

$$\text{Equilibrium Amount} = \text{Initial Amount} + \text{Change in Amount} \quad (6.7.4)$$

$$\text{Equilibrium Amount of } Y = 0.000 \text{ mol} + 0.225 \text{ mol} \quad (6.7.5)$$

$$= +0.225 \text{ mol} \quad (6.7.6)$$

Use the same method to find the equilibrium amount of Z. Convert the equilibrium amounts to concentrations. Recall that the volume of the system is 0.750 liters.

$$[\text{Equilibrium Concentration of Substance}] = \frac{\text{Amount of Substance}}{\text{Volume of System}}$$

$$[X] = \frac{0.350 \text{ mol}}{0.750 \text{ L}} = 0.467 \text{ M}$$

$$[Y] = \frac{0.225 \text{ mol}}{0.750 \text{ L}} = 0.300 \text{ M}$$

$$[Z] = \frac{0.300 \text{ mol}}{0.750 \text{ L}} = 0.400 \text{ M}$$

Use the concentration values to solve the  $K_c$  equation:

$$K_c = \frac{[Y]^3[Z]^4}{[X]^2} \quad (6.7.7)$$

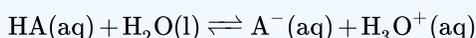
$$= \frac{[0.300]^3[0.400]^4}{[0.467]^2} \quad (6.7.8)$$

$$K_c = 3.17 \times 10^{-3} \quad (6.7.9)$$

### ✓ Example 2: Using an ICE Table with Concentrations

In this example an ICE table is used to find the equilibrium concentration of the reactants and products. (This example will be less in depth than the previous example, but the same concepts are applied.) These calculations are often carried out for weak acid titrations.

Find the concentration of  $A^-$  for the generic acid dissociation reaction:



with  $[HA(aq)]_{\text{initial}} = 0.150 \text{ M}$  and  $K_a = 1.6 \times 10^{-2}$

#### Solution

This equation describes a weak acid reaction in solution with water. The acid (HA) dissociates into its conjugate base ( $A^-$ ) and protons ( $H_3O^+$ ). Notice that water is a liquid, so its concentration is not relevant to these calculations.

#### STEP 1: Fill in the given concentrations

Reaction:	HA	$A^-$	$H_3O^+$
I	0.150 M	0.000 M	0.000 M
C	?	?	?
E	?	?	?

- The contents of the leftmost column are shortened for convenience.

#### STEP 2: Calculate the change concentrations by using a variable 'x'

Reaction:	HA	$A^-$	$H_3O^+$
I	0.150 M	0.000 M	0.000 M
C	-x M	+x M	+x M
E	?	?	?

- The change in concentration is unknown, so the variable x is used to denote the change. x is the same for both products and reactants because equal stoichiometric amounts of  $A^-$  and  $H_3O^+$  are generated when HA dissociates in water.

### STEP 3: Calculate the concentrations at equilibrium

Reaction:	HA	A <sup>-</sup>	H <sub>3</sub> O <sup>+</sup>
I	0.150 M	0.000 M	0.000 M
C	-x M	+x M	+x M
E	0.150 - x M	x M	x M

- To find the equilibrium amounts the I row and the C row are added. Use these values and  $K_a$  (the equilibrium constant for acids) to find the concentration  $x$ .

### STEP 4: Use the ICE table to calculate concentrations with $K_a$

The expression for  $K_a$  is written by dividing the concentrations of the products by the concentrations of the reactants. Plugging in the values at equilibrium into the equation for  $K_a$  gives the following:

$$K_a = \frac{x^2}{0.150 - x} = 1.6 \times 10^{-2}$$

To find the concentration  $x$ , rearrange this equation to its quadratic form, and then use the quadratic formula to find  $x$ :

$$(1.6 \times 10^{-2})(0.150 - x) = x^2$$

$$x^2 + (1.6 \times 10^{-2})x - (0.150)(1.6 \times 10^{-2}) = 0$$

This is the typical form for a quadratic equation:

$$Ax^2 + Bx + C = 0$$

where, in this case:

- $A = 1$
- $B = 1.6 \times 10^{-2}$
- $C = (-0.150)(1.6 \times 10^{-2}) = -2.4 \times 10^{-3}$

The quadratic formula gives two solutions (but only one physical solution) for  $x$ :

$$x = \frac{-B + \sqrt{B^2 - 4AC}}{2A}$$

and

$$x = \frac{-B - \sqrt{B^2 - 4AC}}{2A}$$

Intuition must be used in determining which solution is correct. If one gives a negative concentration, it can be eliminated, because negative concentrations are unphysical.

The  $x$  value can be used to calculate the equilibrium concentrations of each product and reactant by plugging it into the elements in the E row of the ice table.

[Solution:  $x = 0.0416$ ,  $-0.0576$ .  $x = 0.0416$  makes chemical sense and is therefore the correct answer.]

For some problems like example 2, if  $x$  is significantly less than the value for  $K_a$ , then the  $x$  of the reactants (in the denominator) can be omitted and the concentration for  $x$  should not be greatly affected. This will make calculations faster by eliminating the necessity of the quadratic formula.

### Checklist for ICE tables

- Make sure the reversible equation is **balanced** at the start of the problem; otherwise, the wrong amounts will be used in the table.
- The given data should be in **amounts, concentrations, partial pressures**, or somehow able to be converted to such. If it is not, then an ICE table will not help solve the problem.

- If the ICE table has the **equilibrium in amounts**, make sure to convert equilibrium values to concentrations before plugging in to solve for  $K_c$ .
- If the given data is in **amounts or concentrations**, use the ICE table to find  $K_c$ . If the given data is in **partial pressures**, use the ICE table to find  $K_p$ . If you desire to convert from one to the other, remember that

$$K_p = K_c(RT)^{\Delta n_{gas}}$$

It is simpler to use the ICE table with the appropriate givens and convert at the end of the problem.

- Enter in **known data first**, and then calculate the unknown data.
- If there is a **negative value in the "initial" or "equilibrium" rows**, reexamine the calculation. A negative concentration, amount, or partial pressure is physically impossible. Obviously, the "change" row can contain a negative value.
- **Pay attention to the state of each reactant and product.** If a compound is a solid or a liquid, its concentrations are not relevant to the calculations. Only concentrations of gaseous and aqueous compounds are used.
- In the "change" row the values will usually be a variable, denoted by  $x$ . It must first be understood which direction the equation is going to reach equilibrium (from left to right or from right to left). The value for "change" in the "from" direction of the reaction will be the opposite of  $x$  and the "to" direction will be the positive of  $x$  (adding concentration to one side and take away an equal amount from the other side).
- Know the **direction of the reaction**. This knowledge will affect the "change" row of the ICE table (for our example, we knew the reaction would proceed forward, as there was no initial products). Direction of reaction can be calculated using  $Q$ , the reaction quotient, which is then compared to a known  $K$  value.
- It is easiest to **use the same units** every time an ICE table is used (molarity is usually preferred). This will minimize confusion when calculating the equilibrium constants. ICE tables are usually used for weak acid or weak base reactions because all of the nature of these solutions. The amount of acid or base that will dissociate is unknown (for strong acids and strong bases it can be assumed that all of the acid or base will dissociate, meaning that the concentration of the strong acid or base is the same as its dissociated particles).

**Partial pressures** may also be substituted for **concentrations** in the ICE table, if desired (i.e., if the concentrations are not known,  $K_p$  instead of  $K_c$  is desired, etc.). "Amount" is also acceptable (the ICE table may be done in amounts until the equilibrium amounts are found, after which they will be converted to concentrations). For simplicity, assume that the word "concentration" can be replaced with "partial pressure" or "amounts" when formulating ICE tables.

### ? Exercise 6.7.1

0.200 M acetic acid is added to water. What is the concentration of  $H_3O^+$  in solution if  $K_c = 1.8 \times 10^{-6}$  ?

**Answer**

$$5.99 \times 10^{-4}$$

### ? Exercise 6.7.2

If the initial concentration of  $NH_3$  is 0.350 M and the concentration at equilibrium is 0.325 M, what is  $K_c$  for this reaction?

**Answer**

$$1.92 \times 10^{-3}$$

### ? Exercise 6.7.3

How is  $K_c$  derived from  $K_p$ ?

**Answer**

$$K_p = K_c(RT)^{\Delta n} \text{ then solve for } K_c$$

### ? Exercise 6.7.4

Complete this ICE table:

Reaction:	[HA]	[A <sup>-</sup> ]	[H <sub>3</sub> O <sup>+</sup> ]
I	0.650 mol	?	?
C	?	?	?
E	0.250 mol	?	?

Answer

Reaction:	HA	A <sup>-</sup>	H <sub>3</sub> O <sup>+</sup>
I	0.650 mol	0.000 mol	0.000 mol
C	-0.400 mol	+0.400 mol	+0.400 mol
E	0.250 mol	0.400 mol	0.400 mol

### Contributors and Attributions

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