

## Equilibrium Calculations

### 1. Calculating $K_{eq}$ from equilibrium concentrations:

Consider the following equilibrium system:

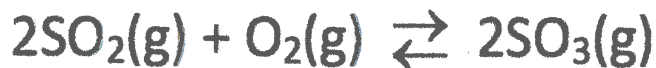


At 200°C, the concentrations of nitrogen, hydrogen and ammonia at equilibrium are measured and found to be  $[\text{N}_2] = 2.12$ ,  $[\text{H}_2] = 1.75$  and  $[\text{NH}_3] = 84.3$ . Determine the value of  $K_{eq}$ .

$$K_{eq} = \frac{[\text{NH}_3]^2}{[\text{N}_2][\text{H}_2]^3} = \frac{(84.3)^2}{(2.12)(1.75)^3} = 625$$

### 2. Calculating concentrations from $K_{eq}$ :

The equilibrium concentrations of  $\text{SO}_2$  and  $\text{O}_2$  are each 0.0500M and  $K_{eq} = 85.0$  at 25°C for the reaction:



Calculate the equilibrium concentration for  $\text{SO}_3$  at this temperature.

$$K_{eq} = \frac{[\text{SO}_3]^2}{[\text{SO}_2]^2[\text{O}_2]}$$

$$[\text{SO}_3]^2 = (K_{eq})([\text{SO}_2]^2[\text{O}_2])$$

$$[\text{SO}_3]^2 = (85.0)(0.05)^2(0.05)$$

$$[\text{SO}_3] = 0.010625 \quad [\text{SO}_3]_{eq} = \underline{0.103\text{M}}$$

### 3. Calculating $K_{eq}$ from initial concentrations:

Suppose that 4.00 moles of HI(g) is placed into a 2.00 L flask at 425°C and reacts to produce H<sub>2</sub> and I<sub>2</sub> according to the equation:



At equilibrium the concentrations of H<sub>2</sub> and I<sub>2</sub> are found to each be 0.214 mol/L. Calculate the value of  $K_{eq}$ .

$$K_{eq} = \frac{[\text{H}_2][\text{I}_2]}{[\text{HI}]^2}$$

*\* Don't use  
x - put in  
#s !!*

$$[\text{HI}]_{\text{initial}} = \frac{4.00 \text{ mol}}{2.00 \text{ L}} = 2.00 \frac{\text{mol}}{\text{L}}$$

$$[\text{H}_2]_{\text{eq}} = [\text{I}_2]_{\text{eq}} = 0.214 \text{ M}$$

⇒ create an ICE table

	$2\text{HI(g)} \rightleftharpoons$	$\text{H}_2\text{(g)} +$	$\text{I}_2\text{(g)}$
Initial	2.00M	0.00M	0.00M
change	-2x	+x	+x
equilibrium	2-2x	x	x

@ equilib  $x = [\text{H}_2] = [\text{I}_2] = 0.214 \text{ M}$

$$[\text{HI}] = 2 - 2(0.214) = 1.57 \text{ M}$$

$$= 1.86 \times 10^{-2}$$

$$K_{eq} = \frac{(0.214)(0.214)}{(1.57)^2}$$



#### 4. Calculating initial concentrations from $K_{eq}$ :

A certain amount of  $\text{NO}_2(\text{g})$  was placed into a 5.00L bulb and reacted according to the equation:



When equilibrium was reached, the concentration of  $\text{NO}(\text{g})$  was 0.800 M. If  $K_{eq}$  has a value of 24.0, how many moles of  $\text{NO}_2$  were originally placed into the bulb?

$$K_{eq} = \frac{[\text{NO}_2]^2}{[\text{NO}]^2[\text{O}_2]}$$

$$[\text{NO}]_{eq} = 0.800\text{M}$$

$$[\text{NO}]_{initial} = y$$

	$2\text{NO}(\text{g})$	$+\text{O}_2(\text{g})$	$\rightleftharpoons$	$2\text{NO}_2(\text{g})$
I	0	0		y
C	+2x	+x		-2x
E	2x	x		y-2x
	$\uparrow$ 0.800M	$\nearrow$ 0.400M		$\rightarrow$ y-0.800M

$$K_{eq} = \frac{[\text{NO}_2]^2}{[\text{NO}]^2[\text{O}_2]}$$

$$24.0 = \frac{(y-0.800)^2}{(0.800)^2(0.400)}$$

$$24.0 = \frac{(y-0.800)^2}{0.256}$$

$$(y-0.800)^2 = (24.0)(0.256)$$

$$(y-0.800)^2 = 6.144$$

$$y-0.800 = 2.479$$

$$y = 3.279\text{M}$$

$[\text{NO}_2]_{initial}$

$$\text{moles NO}_2 = \left(3.279 \frac{\text{mol}}{\text{L}}\right)(5.00\text{L})$$

$$= \boxed{16.4 \text{ mol}}$$

## 5. Determining [equilibrium] from [initial]

$K_{eq} = 3.5$  for the reaction:



If 4.0 mol of  $\text{SO}_2(\text{g})$  and 4.0 mol of  $\text{NO}_2(\text{g})$  are put into a 5.0 L bulb and allowed to come to equilibrium, what concentration of all species will exist at equilibrium?

	$\text{SO}_2(\text{g})$	$\text{NO}_2(\text{g})$	$\text{SO}_3(\text{g})$	$\text{NO}(\text{g})$
I	0.80M	0.80M	0	0
C	-x	-x	+x	+x
E	0.80-x	0.80-x	x	x

$$K_{eq} = \frac{[\text{SO}_3][\text{NO}]}{[\text{SO}_2][\text{NO}_2]}$$

initial  
 $[\text{SO}_2] = [\text{NO}_2] = \frac{4.0 \text{ mol}}{5.0 \text{ L}} = 0.80 \text{ M}$

$$K_{eq} = 3.5 = \frac{x^2}{(0.80-x)^2}$$

$$1.87 = \frac{x}{0.8-x}$$

$$1.87(0.8-x) = x$$

$$1.496 - 1.87x = x$$

$$1.496 = 2.87x$$

$$x = 0.52 \text{ M}$$

at equilib

$$[\text{SO}_3] = 0.52 \text{ M}$$

$$[\text{NO}] = 0.52 \text{ M}$$

$$[\text{SO}_2] = 0.28 \text{ M}$$

$$[\text{NO}_2] = 0.28 \text{ M}$$

## 6. Determining [equilibrium] after a shift

A 1.0 L reaction vessel contained 1.0 mol of  $\text{SO}_2$ , 4.0 mol of  $\text{NO}_2$ , 4.0 mol of  $\text{SO}_3$  and 4.0 mol of  $\text{NO}$  at equilibrium according to the reaction:



If 3.0 mol of  $\text{SO}_2$  are added to the mixture, what will the new concentration of  $\text{NO}$  be when equilibrium is re-established?

$$K_{\text{eq}} = \frac{[\text{SO}_3][\text{NO}]}{[\text{SO}_2][\text{NO}_2]} = \frac{(4.0)(4.0)}{(1.0)(4.0)} = 4.0$$

	$\text{SO}_2$	$\text{NO}_2$	$\text{SO}_3$	$\text{NO}$
I	1.0 + 3.0	4.0	4.0	4.0
C	-x	-x	+x	+x
E	4.0 - x	4.0 - x	4.0 + x	4.0 + x

$$K_{\text{eq}} = \frac{(4.0 + x)^2}{(4.0 - x)^2} = 4.0$$

$$\frac{4.0 + x}{4.0 - x} = 2.0$$

$$4.0 + x = 2(4.0 - x)$$

$$4.0 + x = 8.0 - 2.0x$$

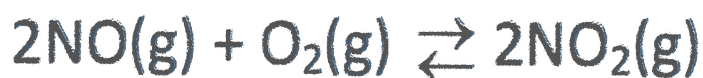
$$3.0x = 4.0$$

$$x = 1.33\text{M}$$

$$[\text{NO}] = 4.0 + 1.33 = \boxed{5.3\text{M}}$$

- for some problems, a numerical answer is NOT required but rather a DECISION must be made
  - > for example . . . which way will the reaction shift in order to reach equilibrium? OR
  - > how will the concentration of reactants and products change in order to reach equilibrium?
- for these decision type problems a **reaction quotient (Q)** or **Trial  $K_{eq}$**  is used

Consider the following equation:



the reaction quotient is:

$$Q = \frac{[\text{NO}_2]^2}{[\text{NO}]^2[\text{O}_2]}$$

- notice that the reaction quotient is the same as the equilibrium expression except that we will use initial concentrations to solve for Q
- our decision will be based on comparing the reaction quotient (Q) to the equilibrium constant ( $K_{eq}$ )

If  $Q = K_{eq}$ , then the system is at **EQUILIBRIUM** and no shift will occur

If  $Q < K_{eq}$ , then  $\frac{[\text{PRODUCTS}]}{[\text{REACTANTS}]}$  is **TOO SMALL** and shift right, more **PRODUCTS**

If  $Q > K_{eq}$ , then  $\frac{[\text{PRODUCTS}]}{[\text{REACTANTS}]}$  is **TOO BIG** and shift left, more **REACTANTS**

## 7. Determining the direction of shift; Trial $K_{eq}$

$K_{eq} = 49$  for the equilibrium:



If 2.0 mol of  $\text{NO}(\text{g})$ , 0.20 mol of  $\text{O}_2(\text{g})$  and 0.40 mol of  $\text{NO}_2(\text{g})$  are put into a 2.0 L bulb, which way will the reaction shift in order to reach equilibrium?

Support your answer with the appropriate calculations.

$$Q = \frac{[\text{NO}_2]^2}{[\text{NO}]^2[\text{O}_2]}$$

$$Q = \frac{(0.20)^2}{(1.0)^2(0.10)} = 0.4$$

$$[\text{NO}] = \frac{2.0 \text{ mol}}{2.0 \text{ L}} = 1.0 \text{ M}$$

$$[\text{O}_2] = \frac{0.20 \text{ mol}}{2.0} = 0.10 \text{ M}$$

$$[\text{NO}_2] = \frac{0.40 \text{ mol}}{2.0 \text{ L}} = 0.20 \text{ M}$$

$Q < K_{eq} \Rightarrow$  need to p. to get bigger  
 $\Rightarrow$  shift to products