Material Shift

Performed BEFORE the I.C.E. Equilibrium Solution

…when a strong/large equilibrium shift is predicted.

Converting Products to Reactants

Converting Reactants to Products

Making equilibrium mathematics more easily solved

Problem 1: $K_c << 1$ **Favors Reactants and only Reactants initially present**
X~0 Assumption valid…No material shift required

Problem 2: $K_c << 1$ **Favors Reactants and only Products initially present**
X~0 Assumption Invalid & Material shift required

Problem 3: $K_c << 1$ **Favors Reactants and only Products initially present**
X~0 Assumption Invalid & Material shift required

Problem 4: $K_c >> 1$ **Favors Products**
and BOTH Products and Reactants are initially present.
X~0 Assumption Invalid & Material shift required

1. No Material Shift Required

1.00 mole of H_2S gas is placed in a closed 2.00 liter container
Assume that no product is originally present and
determine the concentrations of all species after equilibrium is reached.

Reactants!

$$2\ H_2S_{(g)} \leftrightarrow 2\ H_{2(g)} + 1\ S_{2(g)}$$

1.00mol/2.00L SHIFT →

	$2\ H_2S_{(g)}$	$2\ H_{2(g)}$	$1\ S_{2(g)}$
I	**0.500 M**	**0.000 M**	**0.000 M**
C	**-2X**	**+2X**	**+X**
E	**0.500 M – 2X**	**0.000 +2X**	**0.000 +X**

K_C = 1.67×10^{-7}

Small K_C ⇒ Favors Reactants

Initially, only reactants are present.

Shifts *weakly* to the right (products).

CAN use X ~ 0 assumption. ☺

Easy math ahead.

Material Shift NOT REQUIRED

$$\frac{[H_2]^2\ [S_2]}{[H_2S]^2} = \frac{(2X)^2\ X}{(0.500 - 2X)^2} =$$

X = 0

Solve for "X"

$$\frac{4X^3}{(0.500)^2} = 1.67 \times 10^{-7}$$

$$X = 2.18_{54} \times 10^{-3}$$

1. No Material Shift Required

$$2\ H_2S_{(g)} \leftrightarrow 2\ H_{2(g)} + S_{2(g)}$$

$K_C = 1.67 \times 10^{-7}$

	$2\ H_2S_{(g)}$	$2\ H_{2(g)}$	$S_{2(g)}$
E	**0.500M - 2X**	**2X**	**X**

$$X = 2.18_{54} \times 10^{-3}$$

i. Equilibrium Concentrations

$[H_2S]_{eq} = 0.500 - 2X = 0.495_{63}\ M = 0.496\ M$

$[H_2]_{eq} = 2X = 4.37_{08} \times 10^{-3}\ M$

$[S_2]_{eq} = X = 2.18_{54} \times 10^{-3}\ M$

…most of original reactant remains.

…only small amounts of product form.

ii. 5% check

$(0.500 - 2X)^2$

$$\frac{2X}{0.500} \times 100 = 0.87\%$$

$0.87\% < 5\%$

iii. Equilibrium Check

$$\frac{[H_2]^2\ [S_2]}{[H_2S]^2}$$

$$\frac{(4.37_{08} \times 10^{-3})^2\ (2.18_{54} \times 10^{-3})}{(0.496)^2}$$

$= 1.69_{96} \times 10^{-7} = K_C$

2. Material Shift Required

1.00 mole of H_2 gas and 0.500 mole S_2 are is placed in a closed 2.00 liter container
Assume that no H_2S is originally present and
determine the concentrations of all species after equilibrium is reached.

Reactants!

$$2\ H_2S_{(g)} \leftrightarrow 2\ H_{2(g)} + 1\ S_{2(g)}$$

Material Shift ←

	$2\ H_2S_{(g)}$	$2\ H_{2(g)}$	$1\ S_{2(g)}$
Initial Moles	**0.00 moles**	**1.00 mole** *2*	**0.500 mole** *: 1 ratio*
Material Shift	**+1.00 mole**	**- 1.00 mole**	**- 0.500 mole**
Final Moles	**1.00 moles**	**0.00 moles**	**0.00 moles**

K_C = 1.67 × 10^{-7}

Small K_C ⇒ Favors Reactants

Initially, only <u>products</u> are present.

Shifts *strongly* to the left (reactants).

Can't use X ~ 0 assumption.

Nasty math ahead.

Material Shift:
Convert product to reactant

	H_2S	H_2	S_2
Initial	**1.00mol**/2.00L **0.500 M**	**0.000 M**	**0.000 M**

Same as problem 1 previously solved using X ~ 0 assumption.

$[H_2S]_{eq}$ = 0.496M **$[H_2]_{eq}$ = $4.37_{08} \times 10^{-3}$ M** **$[S_2]_{eq}$ = $2.18_{54} \times 10^{-3}$ M**