4. Material Shift Required (Large K_c)

0.250 moles of $N_{2(g)}$, 0.500 moles of $H_{2(g)}$ and 0.100 moles of NH_3 are placed in a 1.50 L closed container.

Determine the concentrations of all species after equilibrium is reached.

Products!

Excess **Limiting**

$$N_{2(g)} + 3\ H_{2(g)} \leftrightarrow 2\ NH_{3(g)}$$

Initial Moles **0.250 moles** **0.500 mole** **0.100 mole**

More Product coming!

NOT A ***1 : 3 ratio***

N_2 Limiting Determination

Mole ratio

$$\frac{0.250\text{ mole }N_2}{1} \times \frac{2\text{ mole }NH_3}{1\text{ mole }N_2} = \boxed{\begin{matrix}0.500\text{ mole }NH_3\\ \textit{Larger} \Rightarrow \textit{Excess}\end{matrix}}$$

H_2 Limiting Determination

Mole ratio

$$\frac{0.500\text{ mole }H_2}{1} \times \frac{2\text{ mole }NH_3}{3\text{ mole }H_2} = \boxed{\begin{matrix}0.333_{33}\text{ mole }H_2S\\ \textit{Smaller} \Rightarrow \textit{Limiting}\end{matrix}}$$

Limiting

Left-over N_2 Determination

Mole ratio

$$\frac{0.500\text{ mole }H_2}{1} \times \frac{1\text{ mole }N_2}{3\text{ mole }H_2} = 0.166_{66}\text{ mole }N_{2\text{ consumed}}$$

$$K_C = 3.70 \times 10^8$$

Large K_C ⇒ Favors Products

Initially, a lot of <u>reactant</u> is present.

<u>Shifts strongly to the right</u> (products).

Adds to the pre- existing 0.100 moles

Can't use X ~ 0 assumption.

Nasty math ahead.

Material Shift:

Convert reactant to product

$$\begin{array}{rl} & 0.250\text{ mole }N_{2\text{ initially}} \\ - & 0.166_{66}\text{ mole }N_{2\text{ consumed}} \\ \hline \text{Left-over }N_2 = & 0.083_{33}\text{ mole }N_{2\text{ leftover}} \end{array}$$

4. Material Shift Required (Large K_C)

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K_C = 3.70×10^8

PRODUCTS!

	Excess		**Limiting**		
	$N_{2(g)}$	+	$3\ H_{2(g)}$	$\leftrightarrow$	$2\ NH_{3(g)}$
Initial Moles	0.250 moles		0.500 mole	Material Shift ➡	0.100 mole
Material Shift	**- 0.166_{66} mole**		**-0.500 mole**		**+ 0.333_{33} mole**
Final Moles	**0.08333 moles**		**0.000 moles**		**0.433_{33} moles**

	0.083_{33} mols/1.50 L	**0.00 mols/1.50 L**	**0.433_{33} mols/1.50 L**
Initial	**0.055_{55} M**	**0.000 M**	**0.288_{88} M**

Since there is no H_2 on the reactant side,

the reaction is shifted as far right as is possible

The X ~ 0 assumption will be valid.

4. Material Shift Required (Large K_C)

0.250 moles of $N_{2(g)}$, **0.500** moles of $H_{2(g)}$ and **0.100** moles of NH_3 are placed in a 1.50 L closed container. Determine the concentrations of all species after equilibrium is reached.

K_C = 3.70 × 10^8

	$N_{2(g)}$	+	3 $H_{2(g)}$	↔	2 $NH_{3(g)}$
I	**0.055_{55} M**		**0.000 M**	SHIFT ←	**0.288_{88} M**
C	+X		+3X		-2X
E	**0.055_{55} + X**		**0.000 +3X**		**0.288_{88} - 2X**

$$\frac{[NH_3]^2}{[N_2]\ [H_2]^3} = \frac{(0.288_{88} \overset{X = 0}{- 2X})^2}{(3X)^3\ (0.055_{55} \underset{X = 0}{+ X})}$$

Solve for "X"

$$= \frac{(0.288_{88})^2}{(3X)^3\ (0.055_{55})} = 3.70 \times 10^8$$

$$X = 5.3_{177} \times 10^{-4}$$

4. Material Shift Required (Large K_C)

0.250 moles of $N_{2(g)}$, 0.500 moles of $H_{2(g)}$ and 0.100 moles of NH_3 are placed in a 1.50 L closed container.

Determine the concentrations of all species after equilibrium is reached.

$$N_{2(g)} + 3\ H_{2(g)} \leftrightarrow 2\ NH_{3(g)}$$

$K_C = 3.70 \times 10^8$

E

$0.055_{55} + X$

Critical X=0

$0.000 + 3X$

$0.288_{88} - 2X$

Less Critical X=0

$$X = 5.31_{77} \times 10^{-4}$$

i. Equilibrium Concentrations

$[N_2]_{eq} = 0.055_{02} + X = 0.055_{55}$ M

$[H_2]_{eq} = 0.00 + 3X = 1.59_{53} \times 10^{-3}$ M

$[NH_3]_{eq} = 0.288_8 - 2X = 0.287_{73}$ M

…most of material shifted product remains.

…only small changes to reactant amounts

ii. 5% check

Most Critical: (0.055 + X)

$$\frac{X}{0.055} \times 100 = 1\ \%$$

$1\% < 5\%$ ☺

iii. Equilibrium Check

$$\frac{[NH_3]^2}{[N_2][H_2]^3}$$

$$\frac{(0.287_{73})^2}{(0.055_{55})(1.59_{53} \times 10^{-3})^3}$$

$= 3.67 \times 10^8 = K_C$ ☺