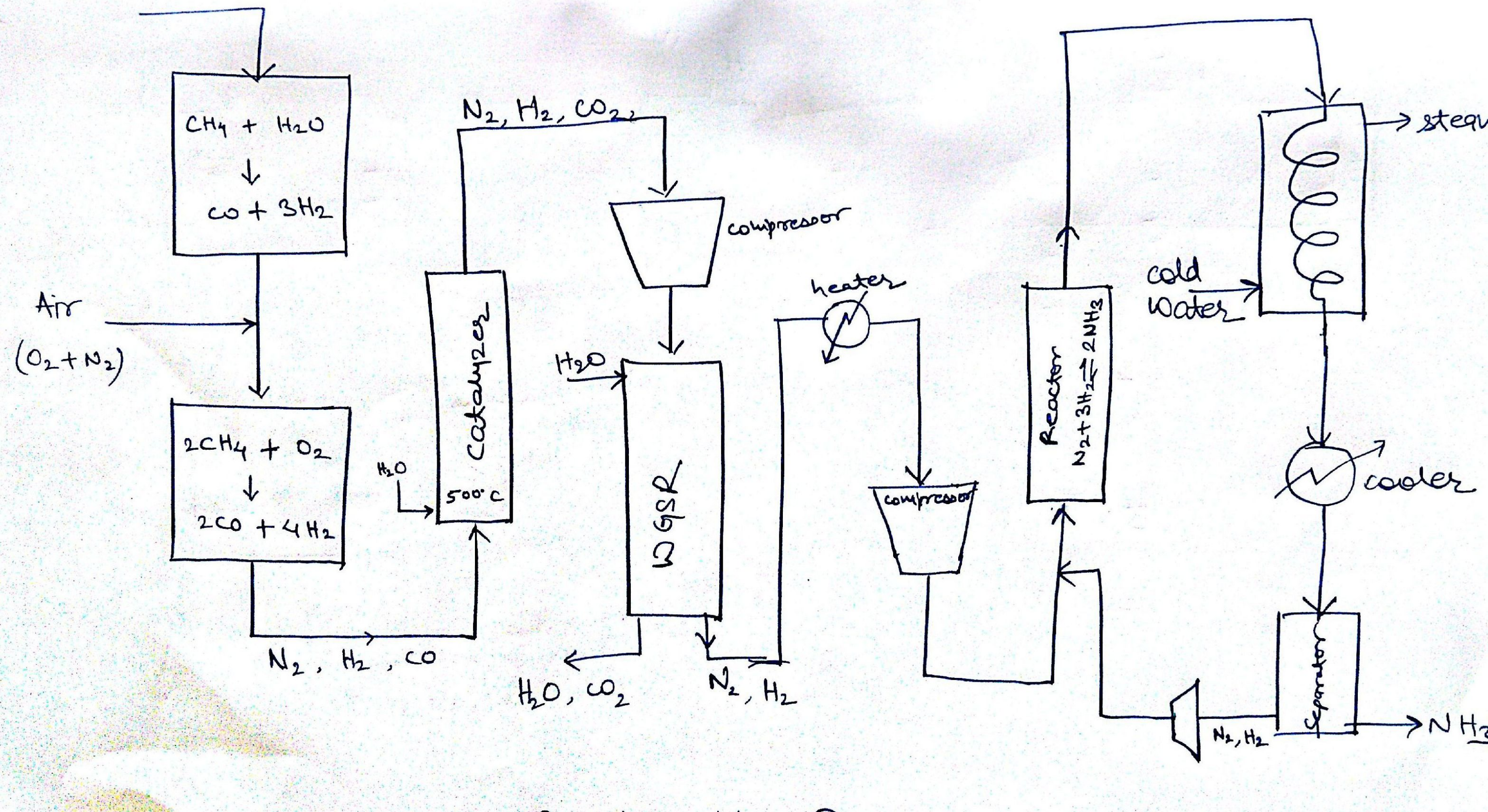
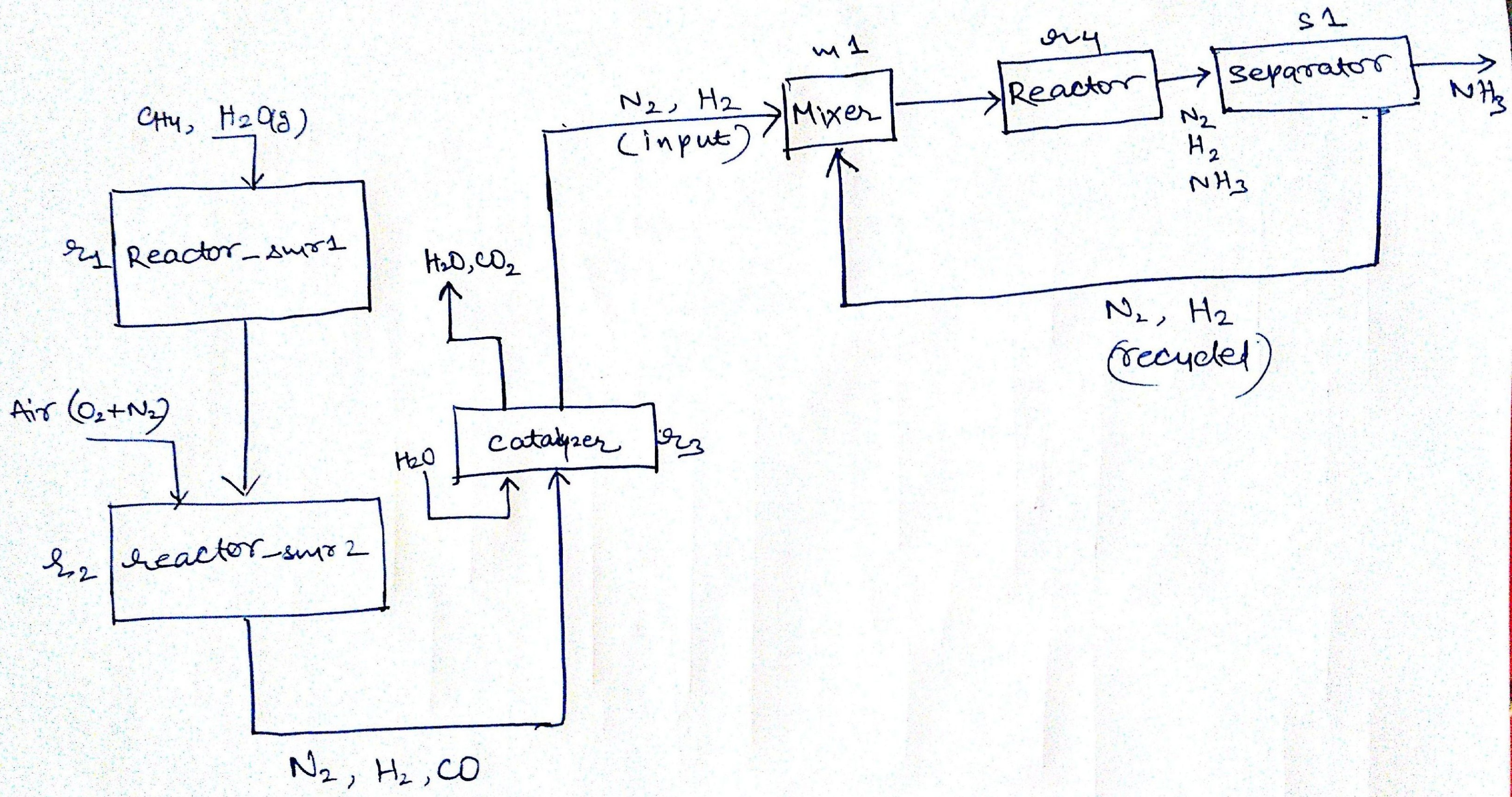


Complete block Diagram



Simplified block diagram for modelling

→ Steam -methane -reactor 1 (SMR 1)

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2$$

$t=0$	a	b	-	-
t	$a-x_4$	$b-x_4$	x_4	$3x_4$

at eqlm, assuming high conversion (~95%)

steam → 0

i.e. $x_4 \approx b$

Unlike normal steam methane reformation, in this, air is fed in step to (not direct O_2), since N_2 is reused in further ammonia production.

hence,

N_2 remains as is (at this step)

and O_2 reacts with CH_4 to convert into CO.

Note:- Assume Air consists of

80% N_2 & 20% O_2

and no other constituents.

→ Steam - Methene-reformation reactor 2 (SMR2)

$$2CH_4 + O_2 \rightleftharpoons 2CO + 4H_2$$

$t=0$	c	d	—	—
t	$c-2x_2 \sim 0$	$d-x_2$	$2x_2$	$4x_2$

$\Rightarrow$ $x_2 = \frac{c}{2}$ and oxygen also is completely consumed

$\Rightarrow$ $d = x_2 = \frac{c}{2}$

Note :- In general, these reactions are high conversion. So assuming ~100% conversion, all the reagents get converted to products.

and,

in-methone & in-oxygen are in their stoichiometric coefficients.

Also input ~~from~~ in SMR2 is nothing but output from SMR 1, so

$$\text{out\_methane}\big|_{SMR1} = \text{in\_methane}\big|_{SMR_2}$$

$$\boxed{a - x_1 = c}$$

Catalyzer

This combines the water gas shift reaction and separation of steam + CO_2 from the mixture.

WGSR :- $CO + H_2O \xrightleftharpoons{100\%\ \text{conversion}} CO_2 + H_2$

	CO	H_2O	CO_2	H_2
t=0	e	f	–	–
t	0 (LR)	f−e	e	e

Here all the carbon-monoxide is consumed completely to given carbon-dioxide and Hydrogen.

Output from catalyzer is

Purge Total	Main Total
$H_2O + CO_2$	$H_2 + N_2$

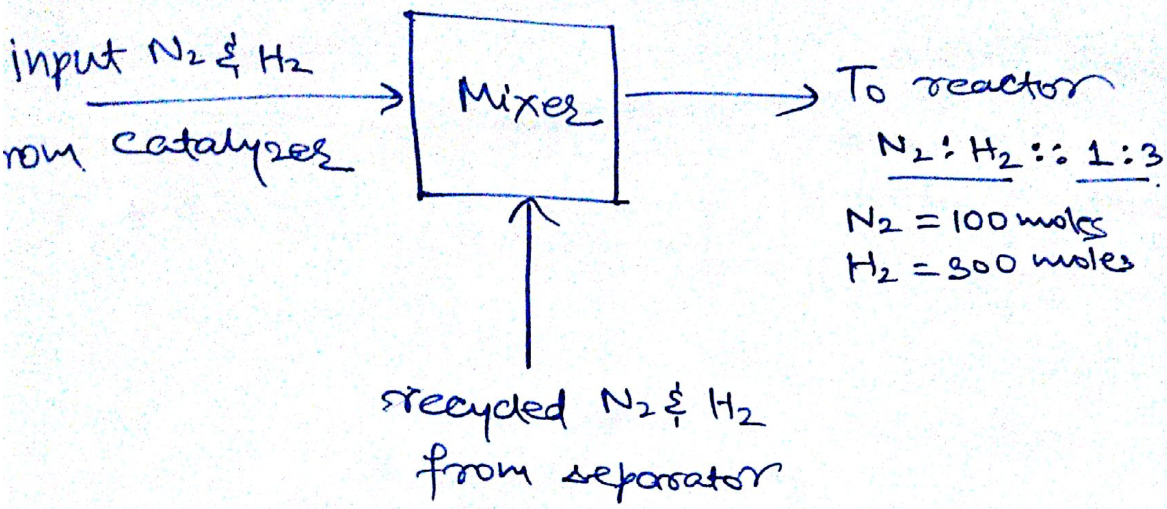
N_2 (not part of the rxn)

This goes into the ammonia reactors.

Note:- At ~~this~~ the mixer stage, this is made sure that H_2 & N_2 are in 3:1.

For our model, we have taken 100 mole of N_2, 300 mole of H_2

Mixer - ammonia



It's job is to simply mix the output from catalyzer and the separated N_2 & H_2 from separator.

Reactor - Ammonia

$$N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)} \quad \Delta H = -92 \frac{kJ}{mol}$$

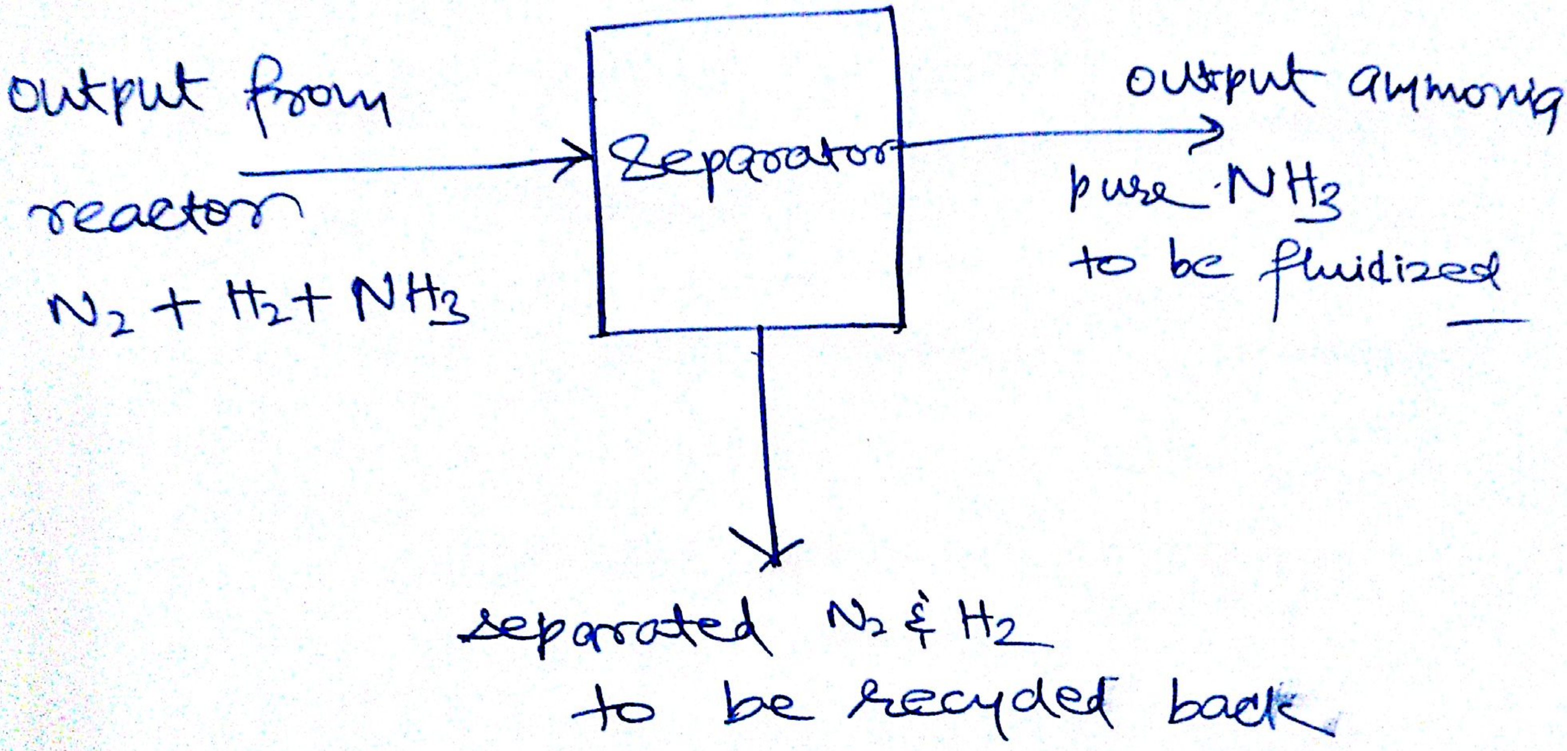
	N_2	$3H_2$	$2NH_3$
$t=0$	100	300	—
$t=t$	$100-x$	$300-3x$	$2x$

According to various journals,

single pass conversion = 15% (for ammonia formation)

hence $x = 15$ moles.

Separator


output from
reactor
$N_2 + H_2 + NH_3$
Separator
output ammonia
pure NH_3
to be fluidized
separated N_2 & H_2
to be recycled back