Reaction and Separation

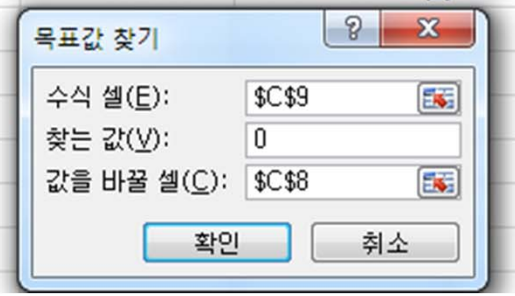
1. Excel을 이용한 수성기체 전환 반응 문제

1단계 – 수식 입력

	A	B	C	D	E
1	A	B	C	D	E
2	Species	Start	End		Mole Fraction
3	CO	1	0.075861343	=B3-$C$8	0.037930672
4	H2O	1	0.075861343	=B4-$C$8	0.037930672
5	CO2	0	0.924138657	=B5+$C$8	0.462069328
6	H2	0	0.924138657	=B6+$C$8	0.462069328
7	Total	2	2.000000	=SUM(C3:C6)	1.0000000
8		Reacting	0.924138657		
9		Equilibrium	0.000233984	=148.4-C5*C6/(C3*C4)	
10		Equation			

2단계 – 목표값 찾기

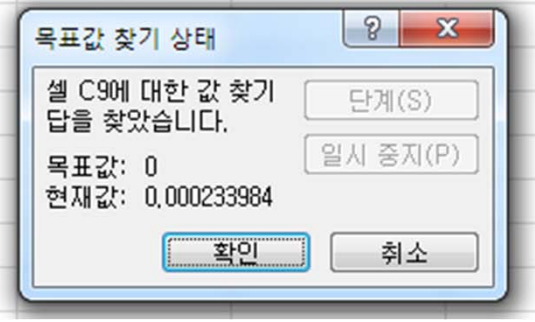
	C	D	E
	C	D	E
	End		Mole Fraction
1	0.075861343	=B3-$C$8	0.037930672
1	0.075861343	=B4-$C$8	0.037930672
0	0.924138657	=B5+$C$8	0.462069328
0	0.924138657	=B6+$C$8	0.462069328
2	2.000000	=SUM(C3:C6)	1.0000000
	0.924138657		
	0.000233984	=148.4-C5*C6/(C3*C4)	



1. Excel을 이용한 수성기체 전환 반응 문제

3단계 – 목표값 찾기

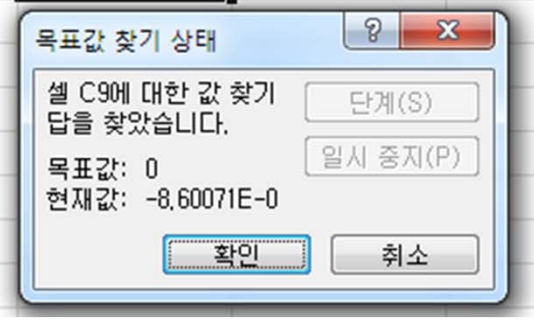
	A	B	C	D	E
1	A	B	C	D	E
2	Species	Start	End		Mole Fraction
3	CO	1	0.075861343	=B3-$C$8	0.037930672
4	H2O	1	0.075861343	=B4-$C$8	0.037930672
5	CO2	0	0.924138657	=B5+$C$8	0.462069328
6	H2	0	0.924138657	=B6+$C$8	0.462069328
7	Total	2	2.000000	=SUM(C3:C6)	1.0000000
8		Reacting	0.924138657		
9		Equilibrium	0.000233984	=148.4-C5*C6/(C3*C4)	
10		Equation			
11					
12					
13					
14					
15					
16					



1. Excel을 이용한 수성기체 전환 반응 문제

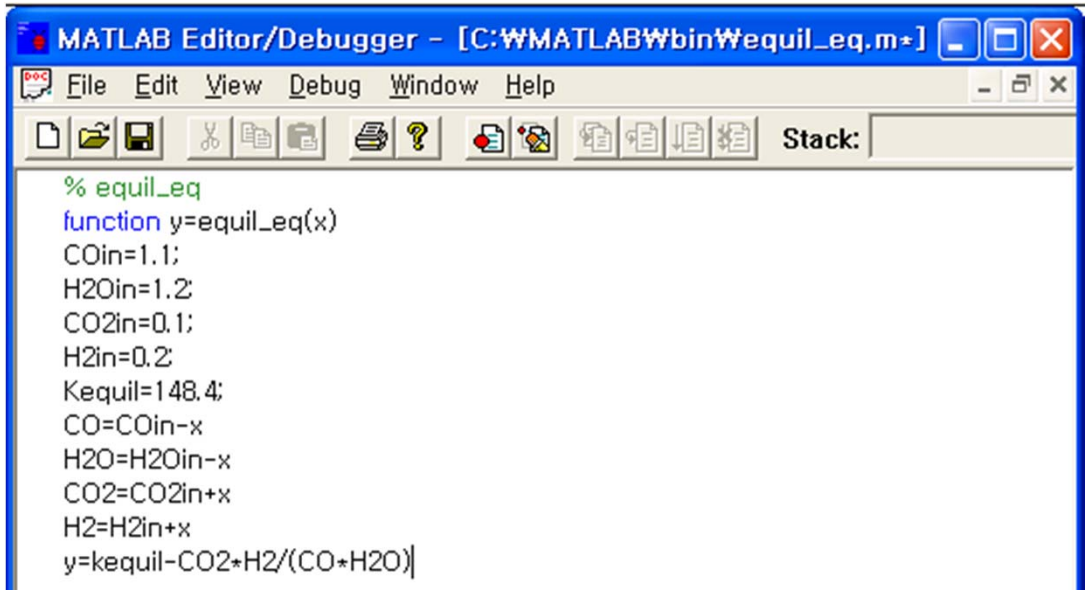
4단계 – Nonstoichiometric Input(각 몰을 1 1.8 0.3 0.1)

	A	B	C	D	E
1	A	B	C	D	E
2	Species	Start	End		Mole Fraction
3	CO	1	0.011641541	=B3-$C$8	0.003637982
4	H2O	1.8	0.811641541	=B4-$C$8	0.253637982
5	CO2	0.3	1.288358459	=B5+$C$8	0.402612018
6	H2	0.1	1.088358459	=B6+$C$8	0.340112018
7	Total	3.2	3.200000	=SUM(C3:C6)	1.0000000
8		Reacting	0.988358459		
9		Equilibrium	-8.60071E-06	=148.4-C5*C6/(C3*C4)	
10		Equation			
11					
12					
13					
14					
15					
16					

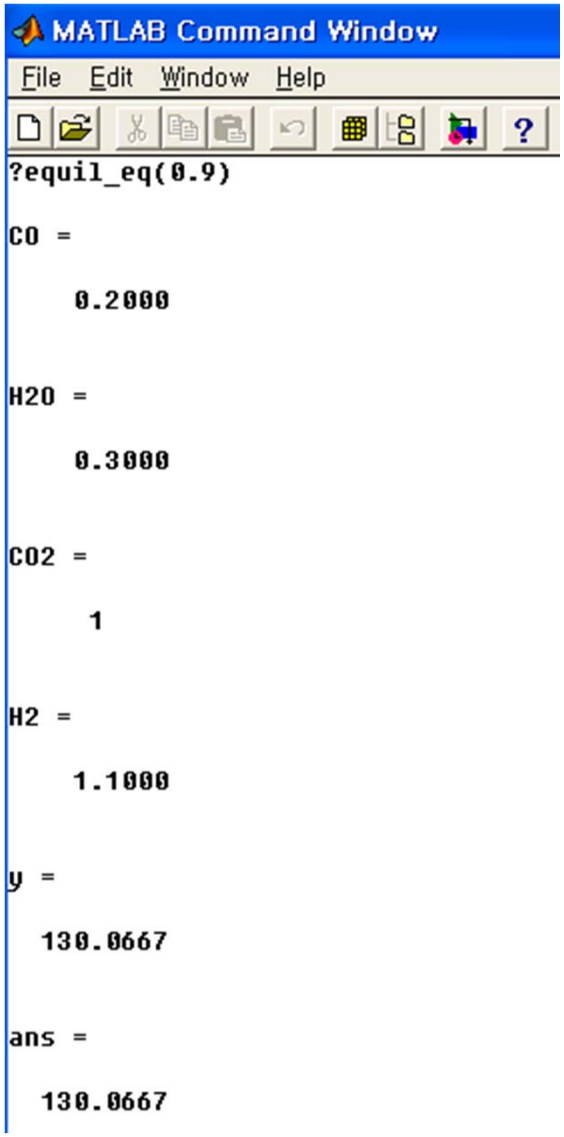


2. MATLAB을 이용한 수성기체 전환 반응 문제

1단계 – m-file 만들기(equil_eq.m)

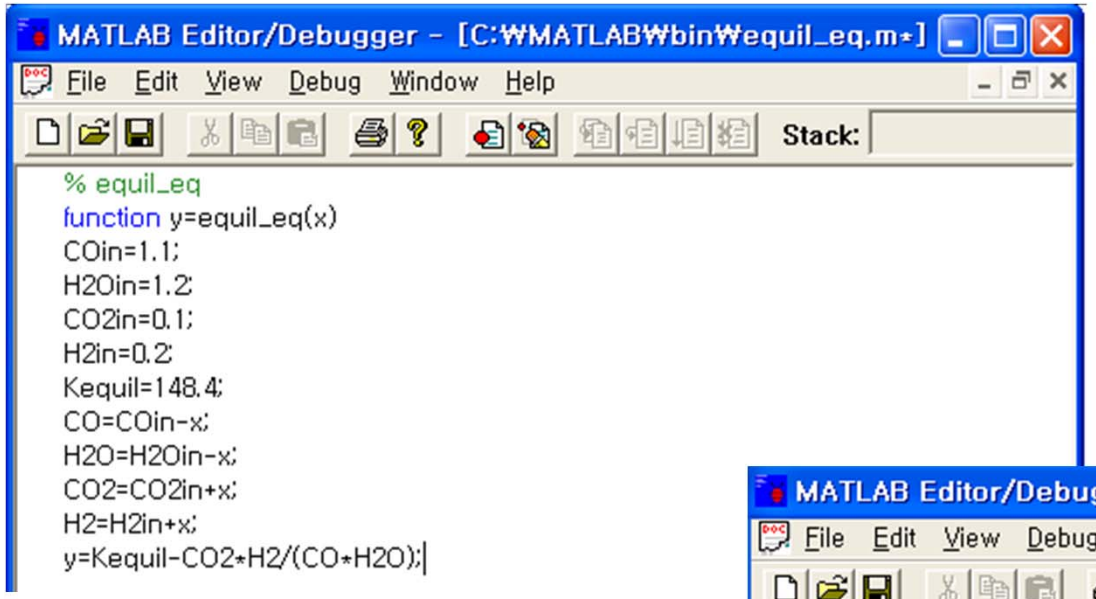


2단계 – 답 구하기

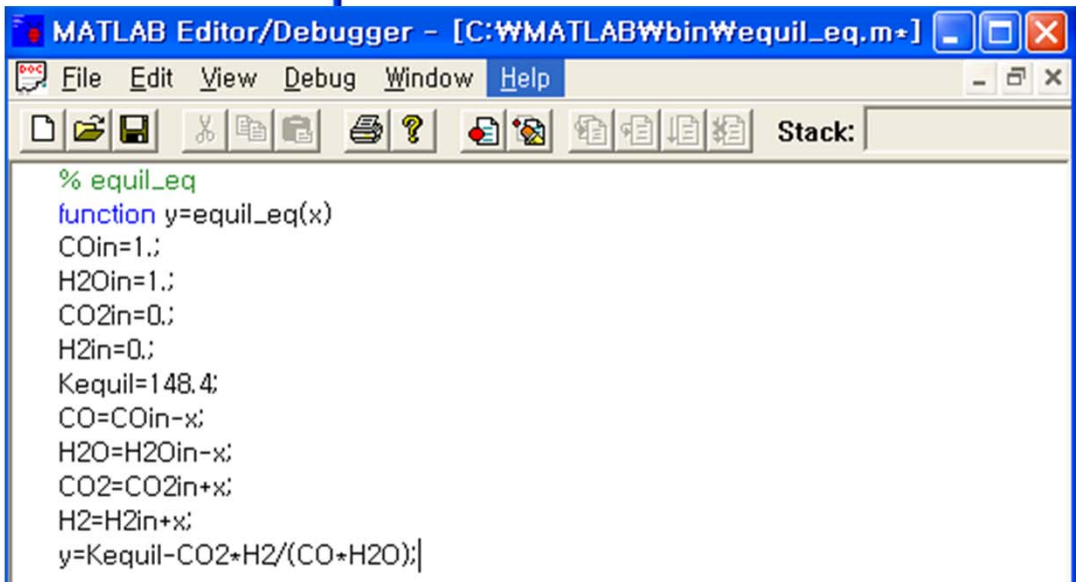


2. MATLAB을 이용한 수성기체 전환 반응 문제

3단계 – m-file에 ' ; ' 삽입하기

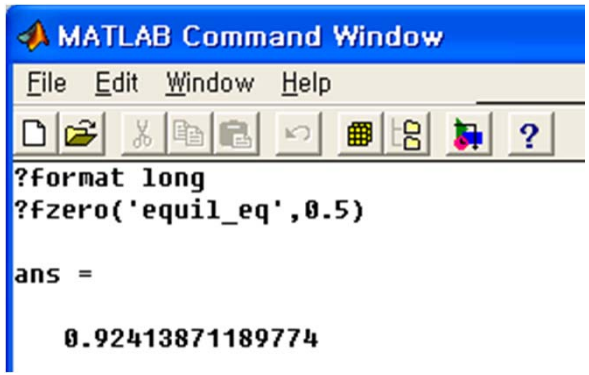


4단계 – Table 4.1로 변형하기

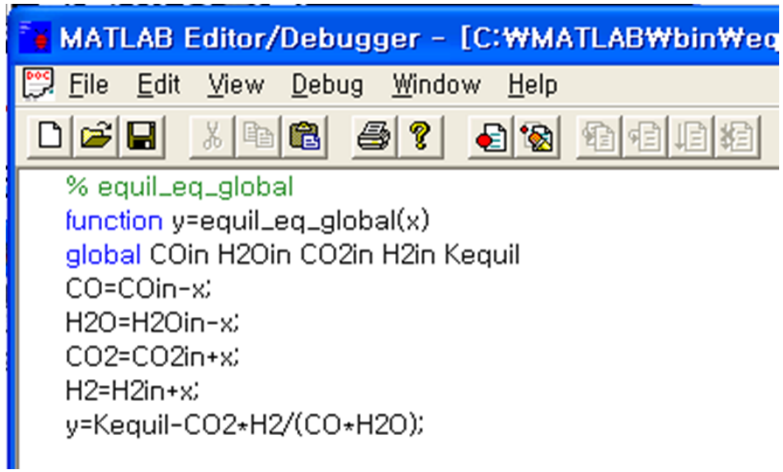


2. MATLAB을 이용한 수성기체 전환 반응 문제

5단계 – 답 구하기



6단계 – m-file 만들기(Nonstoichiometric Input)



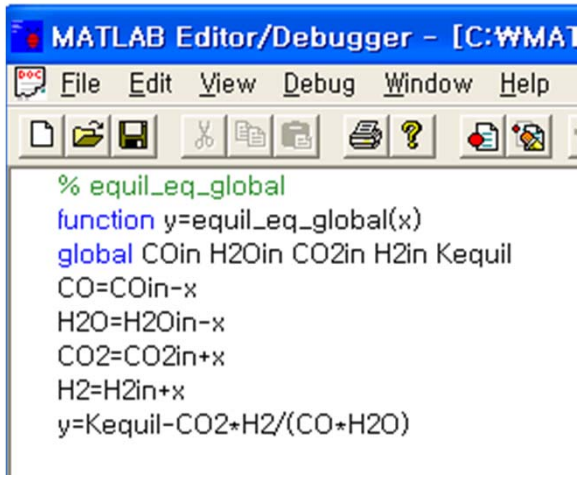
2. MATLAB을 이용한 수성기체 전환 반응 문제

7단계 – 답 구하기

```
?%run equil_eq_global
global COin H2Oin CO2in H2in Kequil
COin=1
H2Oin=1
CO2in=0
H2in=0
Kequil=148.4
x=fzero('equil_eq_global',0.5)

COin =

     1


H2Oin =

     1


CO2in =

     0


H2in =

     0


Kequil =

    1.484000000000000e+002


x =

   0.92413871189774
```

2. MATLAB을 이용한 수성기체 전환 반응 문제

8단계 – m-file 만들기(';'를 삭제)

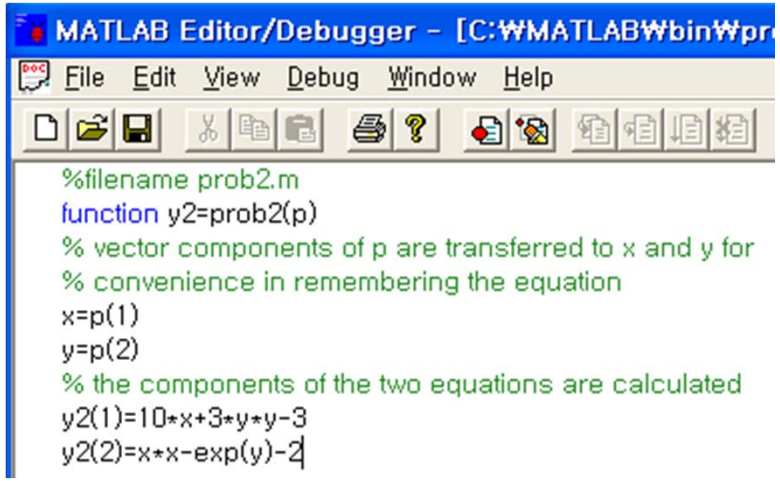


9단계 – 답 구하기

```
H2 =

    0.9241


y =

  3.9790e-013


CO =

    0.0759


H2O =

    0.0759


CO2 =

    0.9241


H2 =

    0.9241


y =

 -1.4495e-012


x =

    0.9241
```

3. MATLAB을 이용한 여러 변수 연립방정식

1단계 – m-file 만들기(prob2.m)

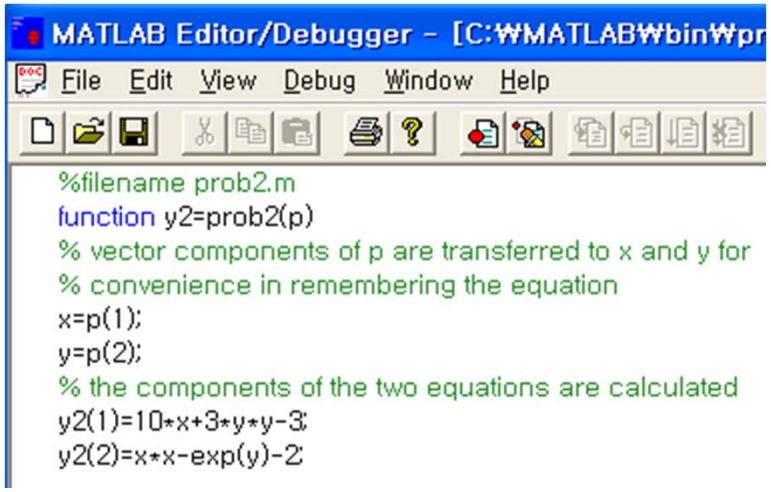


2단계 – 답 구하기

```
?p=[1.5 2.5]

p =

    1.5000    2.5000

?feval('prob2',p)

x =

    1.5000


y =

    2.5000


y2 =

   30.7500


y2 =

   30.7500  -11.9325


ans =

   30.7500  -11.9325
```

3. MATLAB을 이용한 여러 변수 연립방정식

3단계 – 초기 추정값 p0를 이용하여 fsolve를 입력한다.(';' 삽입한다)



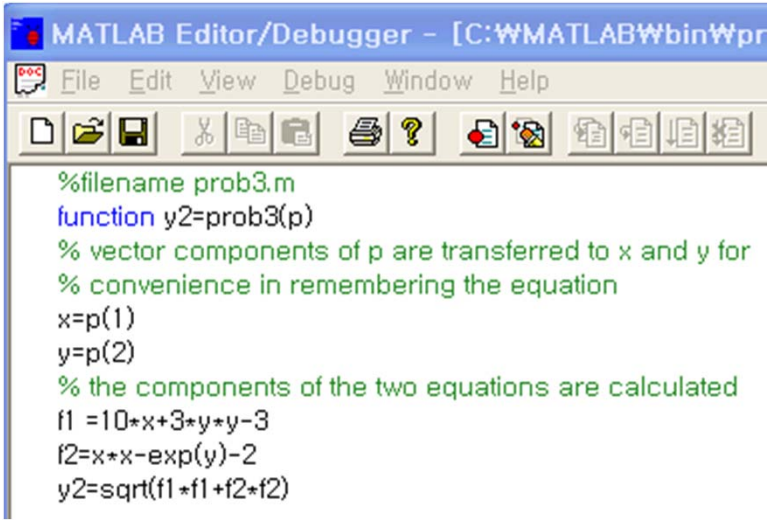

```
?p0=[0 0]

p0 =

     0     0

?z=fsolve('prob2',p)

z =

   -1.4455   -2.4122
```

4단계 – 답 구하기

```
?ans=feval('prob2',z)

ans =

  1.0e-004 *

    0.6378   -0.3016
```

4. MATLAB을 이용한 여러 변수 연립방정식(fminsearch 함수 사용)

1단계 – m-file 만들기(prob3.m)



2단계 – 답 구하기

```
?p0=[0 0]

p0 =

     0     0

?feval('prob3',p)

x =

    1.5000


y =

    2.5000


f1 =

   30.7500


f2 =

  -11.9325


y2 =

   32.9840


ans =

   32.9840
```

4. MATLAB을 이용한 여러 변수 연립방정식(fminsearch 함수 사용)

3단계 – m-file 만들기(';'삽입하고, 초기 추정값[1 1]로 부터 계산) – MATLAB 버전 변경(2010a)

```
1     %filename prob3.m
2     function y2=prob3(p)
3     % vector components of p are transferred to x and y for
4     % convenience in remembering the equation
5     x=p(1)
6     y=p(2)
7     % the components of the two equations are calculated
8     f1=10*x+3*y*y-3
9     f2=x*x-exp(y)-2
10    y2=sqrt(f1*f1+f2*f2)
```

```
>> p0=[1 1]

p0 =

     1     1

>> xvec=fminsearch('prob3',p0)

xvec =

   -1.4456   -2.4122
```

4단계 – 답 구하기(';'를 제거하고 함수 계산)

```
>> ans=feval('prob3',xvec)

f1 =

 -1.0120e-004


f2 =

  5.1047e-006


ans =

  1.0133e-004
```

4. MATLAB을 이용한 여러 변수 연립방정식(fminsearch 함수 사용)

5단계 – m-file 만들기(format long 명령문 사용)

```
>> format long
>> options=optimset('TolFun',1e-12)

options =

                  Display: []
              MaxFunEvals: []
                  MaxIter: []
                   TolFun: 1.000000000000000e-012
```

```
>> xvec=fminsearch('prob3',p0,options)

xvec =

  -1.445552368804647  -2.412158348039360
```

6단계 – 답 구하기(';'를 제거하고 함수 계산)

```
>> feval('prob3',xvec)

f1 =

    1.453059894629405e-012


f2 =

   -9.099387909827783e-013


ans =

    1.714459582701096e-012
```

1. Excel을 이용한 물질수지식(암모니아 공정)

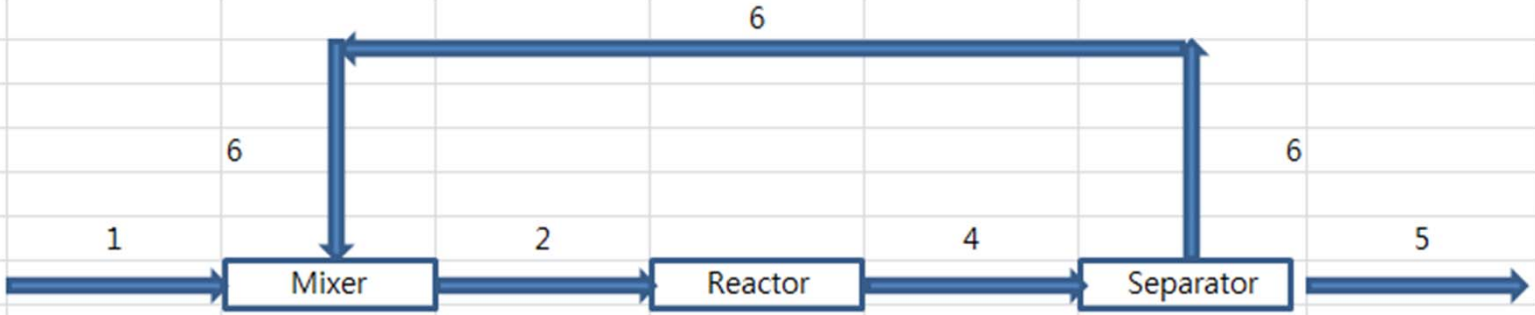
1단계 – 수식 입력(Stream1과 6을 합쳐 Stream2에 주입)

2-4단계 – Stream3의 Nitrogen은 Stream2의 질소에 전환율을 곱하고, Hydrogen은 Nitrogen의 3배, Ammonia는 2배로 설정한다. 반응물은 음수, 생성물은 양수로 표시한다.

5단계 – Stream4는 Stream2와 3의 합

6단계 – Stream5는 98% Ammonia, 5% Nitrogen, Hydrogen은 Nitrogen의 3배

7단계 – Stream6은 각각 Nitrogen의 2배와 3배로 표시한다.

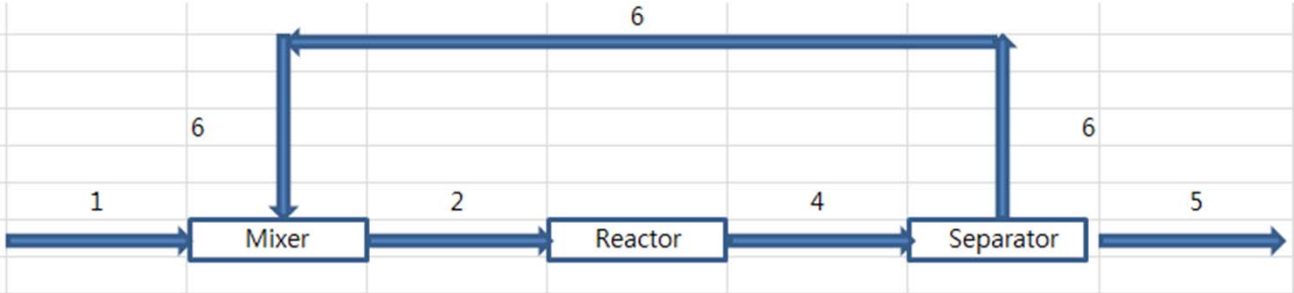


	1	2	3	4	5	6
Nitrogen	100.00	394.09	-98.52	295.57	1.48	294.09
Hydrogen	300.00	1182.27	-295.57	886.70	4.43	882.27
Ammonia	0.00	4.02	197.04	201.07	197.04	4.02
Total	400.00	1580.38	-197.04	1383.33	202.96	1180.38
		Conversion	0.25			

2. Excel을 이용한 물질수지식(평형전환율이 있는 암모니아 공정)

1단계 – 수식 입력

2단계 – 목표값 찾기(Conversion값을 변화시켜 Equation의 값을 0으로 만드는 것) – 해찾기를 이용



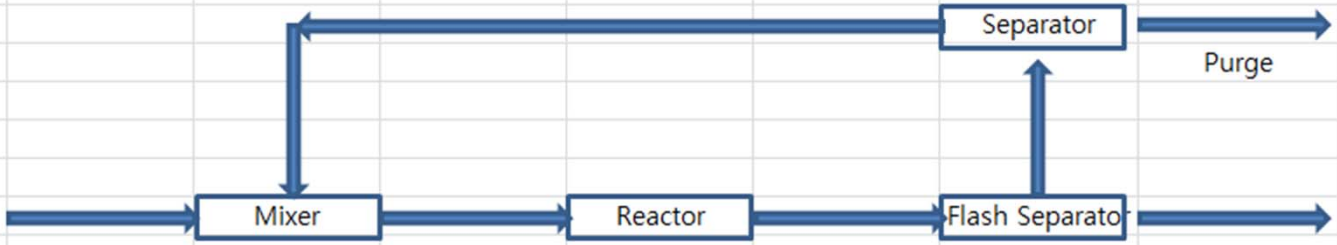
	1	2	3	4	5	6
Nitrogen	100.00	134.83	-99.83	35.00	0.18	34.83
Hydrogen	300.00	404.48	-299.48	105.01	0.53	104.48
Ammonia	0.00	4.07	199.65	203.72	199.65	4.07
Total	400.00	543.38	-199.65	343.73	200.35	143.38

Conversion	0.74039096		
mole fraction our of reactor			
Nitrogen	0.101829904	=F14/$F$17	
Hydrogen	0.305489711	=F15/$F$17	
Ammonia	0.592680385	=F16/$F$17	
Total	1.000000000		
Kp	0.05		
P	220		
Equation	5.38782E-07	=F26-F23/((F21*F22^3)^0.5*F27)	

3. Excel을 이용한 물질수지식(상평형이 있는 암모니아 공정)

1단계 – 수식 입력

2단계 – 목표값 찾기(v값을 변화시켜 f(v)의 값을 0으로 만드는 것) - 해찾기를 이용



	Inlet		Out of Mixer	Reacting	Out of reactor		Product	
	Inlet	Recycle	Out of mixer	Reacting	Out of reactor	Recycle out of flash separator	Product out of flash separator	Purge
Nitrogen	100.00	270.80	370.80	-92.70	278.10	273.54	4.56	2.7354
Hydrogen	300.00	1968.51	2268.51	-278.10	1990.41	1988.39	2.02	19.8839
Ammonia	0.00	115.54	115.54	185.40	300.00	116.70	183.30	1.1670
CO2	1.00	3.80	4.80	0.00	4.80	3.84	0.96	0.0384
Total	400.00	2354.84	2754.84	-185.40	2568.51	2378.63	189.88	23.7863
		Conversion	0.25		v=	0.925839397		
				term1=	term2=			
	zi		K-value	(ki-1)zi	(ki-1)v+1	Ratio	xi	yi
Nitrogen	0.1083	=G14/$G$18	4.8	0.41143729	4.51818971	0.091062421	0.023963795	0.115026216
Hydrogen	0.7749	=G15/$G$18	79	60.44435860	73.21547300	0.825568095	0.010584206	0.836152302
Ammonia	0.1168	=G16/$G$18	0.051	-0.11084259	0.12137841	-0.913198528	0.962274529	0.049076001
CO2	0.0019	=G17/$G$18	0.32	-0.00127159	0.37042921	-0.003432753	0.005048166	0.001615413
Total	1.0019				f(v)=	-0.00000077	1.00187070	1.00186993