Energy Analysis of CO_2 Separation Process with Hollow Fiber Membrane Using ASPEN Simulation Method

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Capture – Membranes (2)

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Background

- Carbon Dioxide (CO_2)
  - Major source of greenhouse gas from Power Plant & Industrial Process
  - CO_2 Emission : Korea ranked 10th in the world
  - Kyoto Protocol : Expected to add carbon tax, emission trade

- For sustainable development, Korea must prepare for the duty for reduction of CO_2 emission.

- Methods of CO_2 separation : Absorption, Adsorption, Membrane
  - Absorption : Low conc. CO_2 recovery process & large scale
    Commercial plant / Blazing of absorbent, Leakage
  - Adsorption : High conc. CO_2 recovery process & middle scale
    Short lifetime of adsorbent
  - <u>Membrane</u> : More environmental-friendly than absorption
    High conc. CO_2 recovery process & small scale
    Need to construct commercial plant in Korea

Purpose of the study

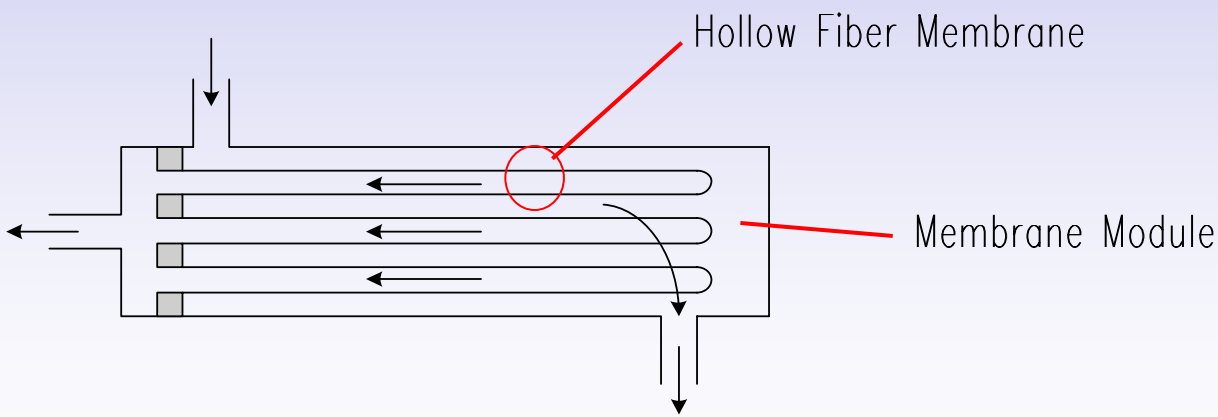
- Perform simulation of CO_2 separation process with hollow fiber membrane by ASPEN plus & Excel.

Scale : 1,000 Nm^3/day of LNG Flue Gas
Target Recovery rate : 90%
Purity of CO_2 : 99%

- It is possible to analyze the actual process including unit equipments, and obtain optimum operation parameters of product or intermediate.
  ex) pressure, temperature, enthalpy, flow, composition etc

- Evaluating energy analysis of CO_2 separation process and calculating cost of operation are required for CO_2 separation & recovery.

Schematic of Hollow Fiber Membrane



Simulation & Analysis Method (1/2)

- **Operating Conditions**

1) Composition of LNG Flue Gas

Composition	Vol %	Wt %
N_2	71.3	72.2
O_2	1.7	2.0
CO_2	8.8	13.9
H_2O	18.2	11.0
Total	100	100

2) Parameters of Hollow Fiber Membrane

Parameter	Amount	Parameter	Amount
P_1 (atm)	6	Num of HF	16,000
P_2 (atm)	0.1	Feed rate	1000 m^3/day
Selectivity [CO_2/N_2]	20	Length of HF	50 cm
Permeability [CO_2]	60 GPU	Pressure ratio (P_2/P_1)	0.167

Simulation & Analysis Method (2/2)

Initial Input Parameters for Membrane Module

- Permeability (Barrer)
- Selectivity(CO_2/N_2)
- Thickness of Selective layer (mm)

• **Initial Input Parameters for Variables of Process**

- Pressure Ratio(R) : P_{feed} / P_{perm}
- Stage-cut : Q_{feed} / Q_{perm}
- Operating Temperature
- Plasticizing

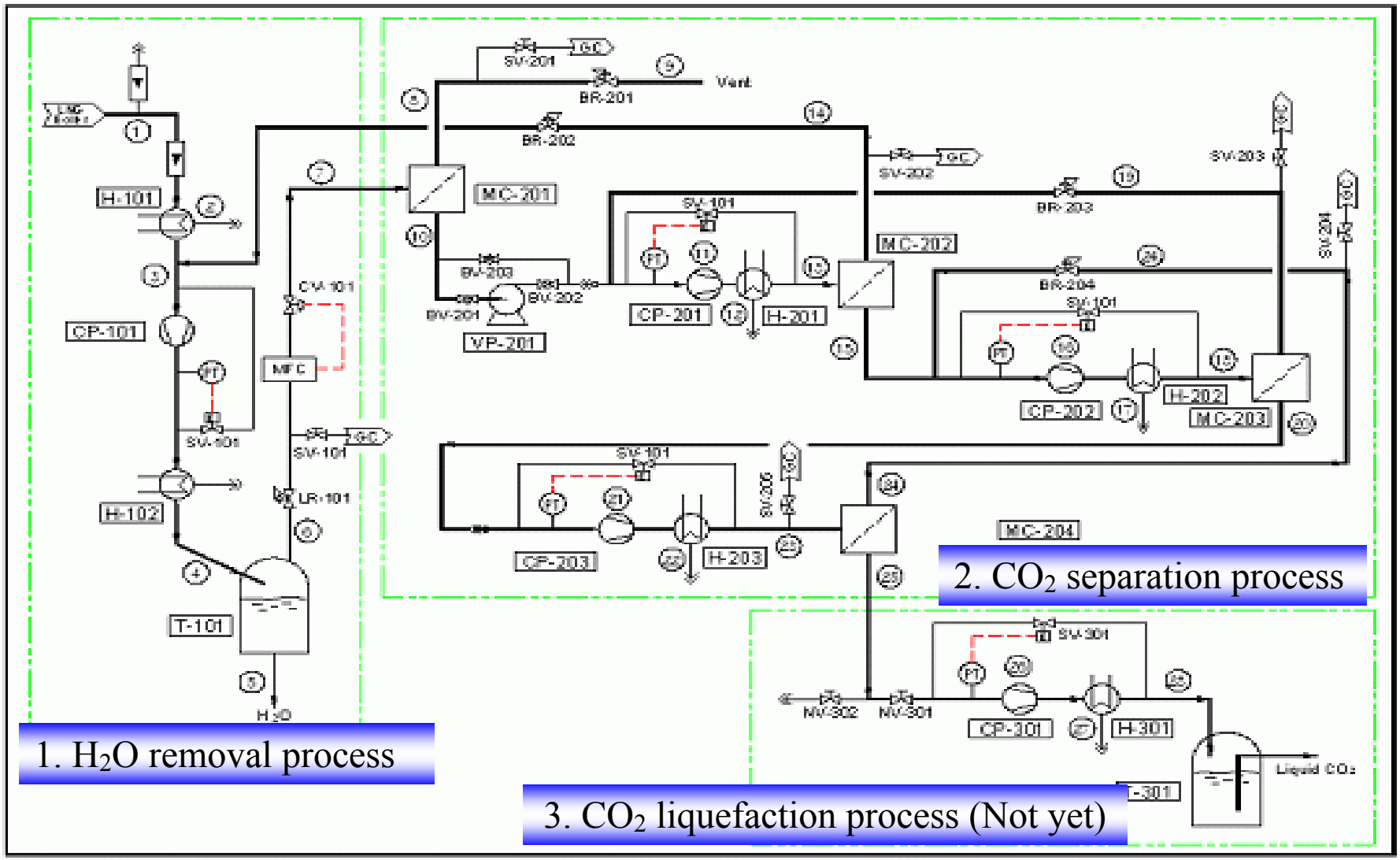
• **Final Results**

- Volume of Permeate (V_P)
- Volume of Retentate (V_R)
- CO_2 Purity at Permeate
- CO_2 Recovery (%)
- Required Surface Area of Membrane (A)
- Required amount of Membrane Module (n)

• Operating Conditions → Simulation for CO_2 Separation Process (Supplement of Membrane Model with Excel in ASPEN code) → Simulating Results → Finding Optimal Conditions → Energy Analysis by Exergy Method → Calculating Capital Cost

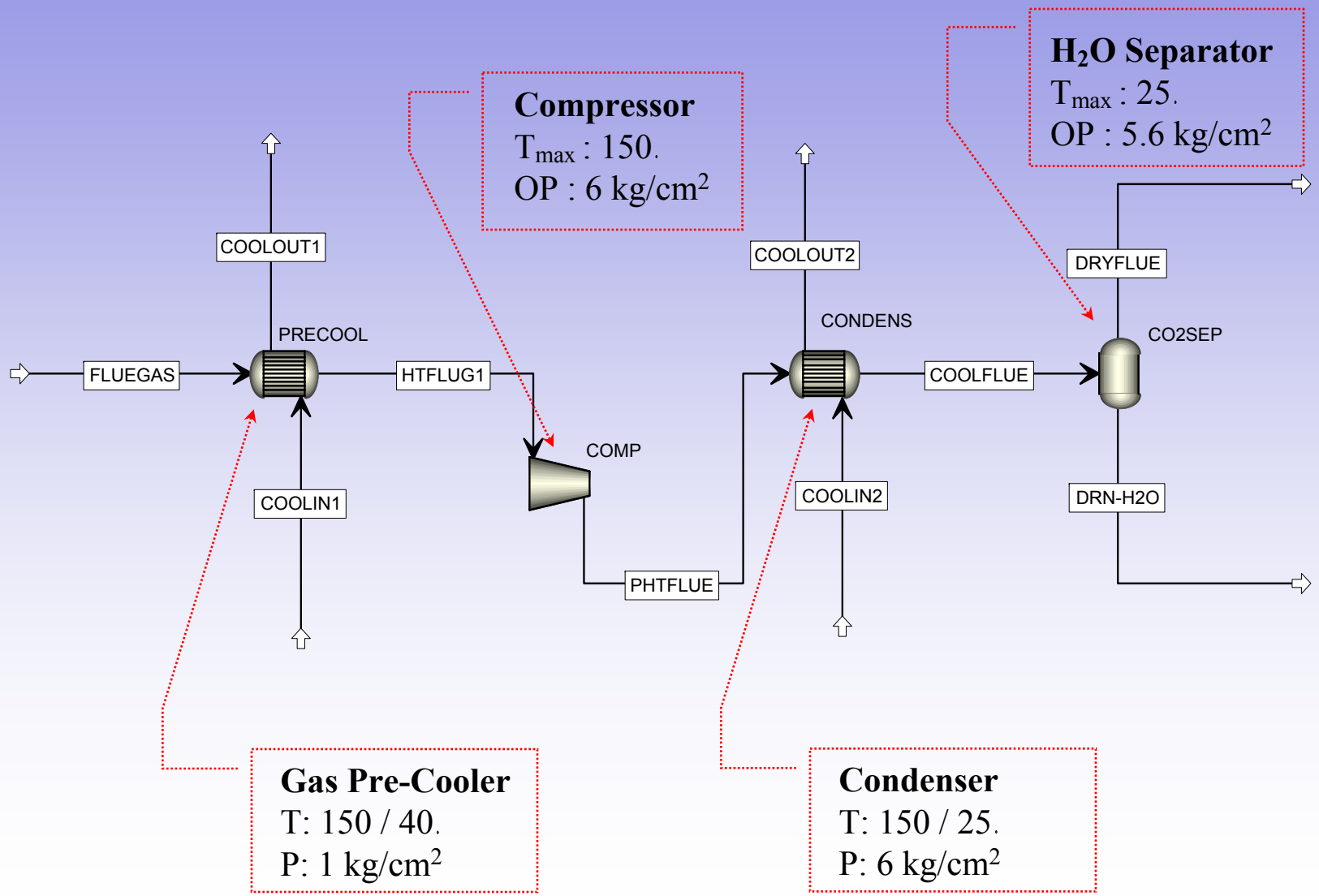
Schematic of Process

- Evaluated CO_2 Separation Plant (Capacity: real exhaust gas, 1000 Nm^3/day) at the Korea Research Institute of Chemical Technology (KRICT)



Simulation of H2O Removal Process

- Simulation of H_2O Removal Process by ASPEN code



Simulation of H2O Removal Process

- Feed rate of dry flue gas : 1000m^3/day (with H2O : 1205m^3/day)
- Composition of feed gas (Volume %)
  - CO_2 : 10%
  - N_2 : 73%
  - H_2O : 17%
- Method of gas property calculation : SRK, Peng-Robinson, RK-Soave

Simulation of H2O Removal Process

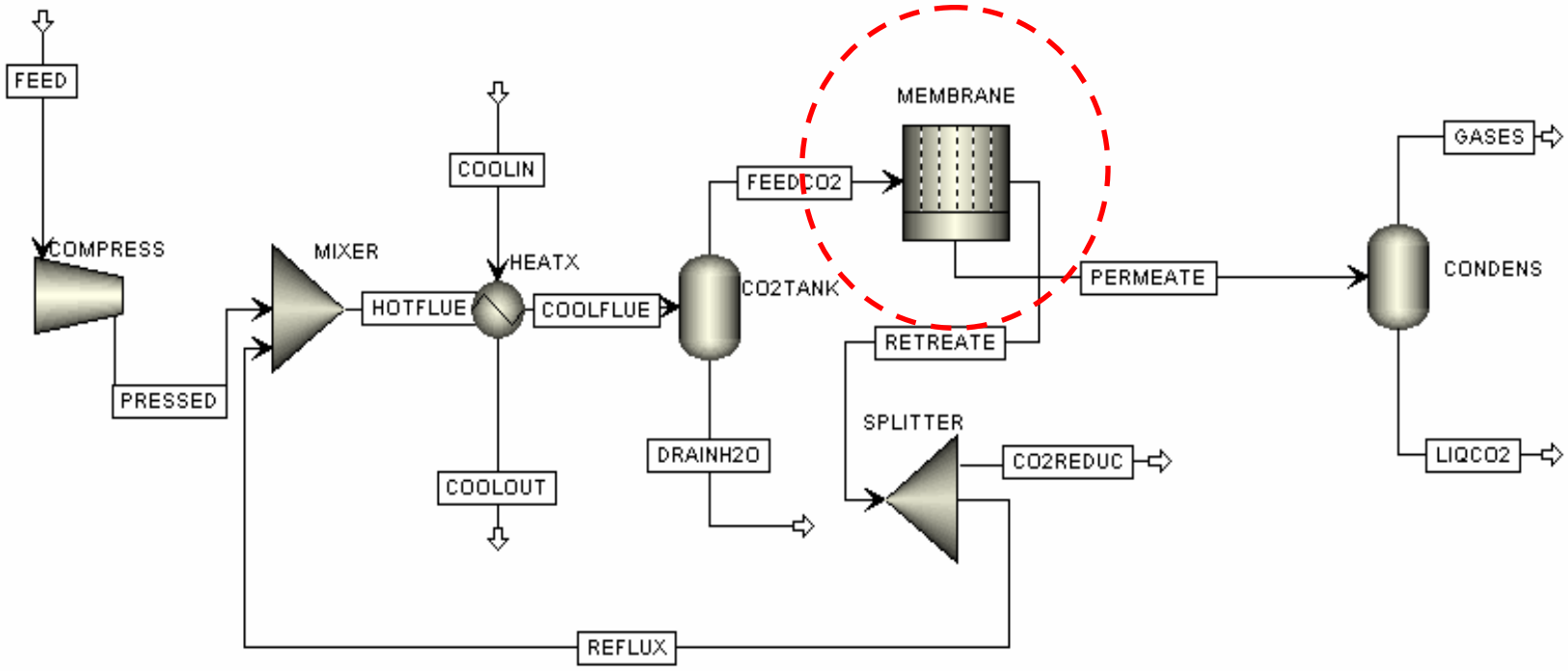
- H2O Composition at 0.(=32F)

1. SRK
   Vol-fraction : 0.1357%
   Mole-fraction : 0.4016%

2. Peng-Robinson
   Vol-fraction : 0.1308%
   Mole-fraction : 0.3871%

3. RK-Soave
   Vol-fraction : 0.1567%
   Mole-fraction : 0.4634%

Simulation of 1 Membrane Module



Simulation of 1 Membrane Module

- Governing Equation of Separation Mechanism in Membrane

$$(\alpha - 1) y_i^2 + \left(1 - \alpha - \frac{1}{R} - \frac{x(\alpha - 1)}{R}\right) y_i + \frac{\alpha x}{R} = 0$$

$$A = \frac{(Vy)_{out}}{(J_A)_{out}} = \frac{(Vy)_{out}}{Q_A (P_1 x - P_2 y_i)_{ave}}$$

$$= \frac{(Vy)_{out}}{Permeate\ flux \times (x - R y_i)_{ave}}$$

α : selectivity

x : Feed composition

y_i: Permeate composition

P_1: Feed Pressure

P_2: Permeate Pressure

R : Pressure ratio(P_2 / P_1)

V : Permeate rate

A : membrane area

Simulation of 1 Membrane Module

1. Simulation with variation of operating parameter
   1) Fix x_T as 0.01
      Fix CO_2 conc. Of Retreate
      Then calculate membrane area, flux and conc. of Permeate with variation of pressure
      2) Fix Pressure
      Fix Pressure,
      Then calculate, **flux and conc. of** Permeate and xT with variation of number of module

2. Simulation with variation of membrane property

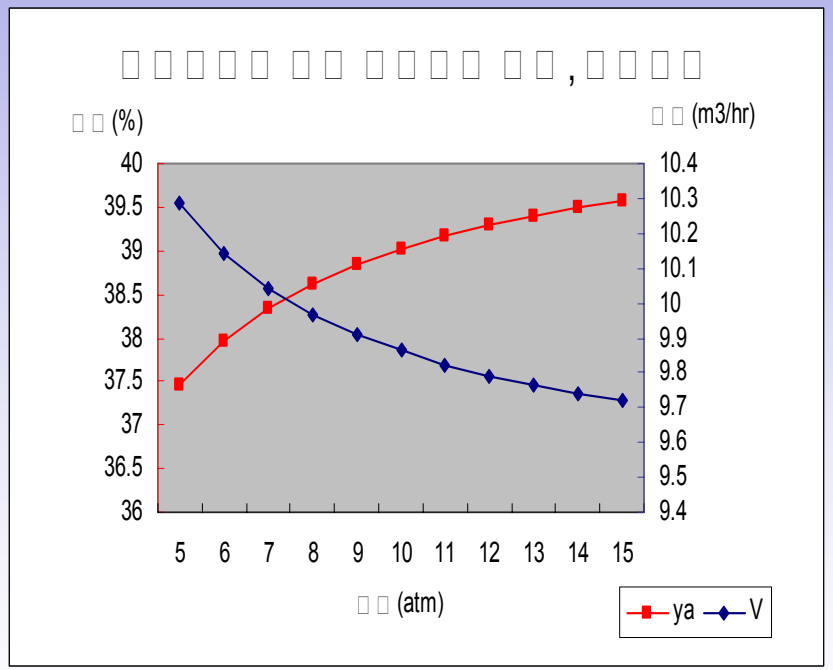
1) Fix permeability as 20, then change selectivity 20~100

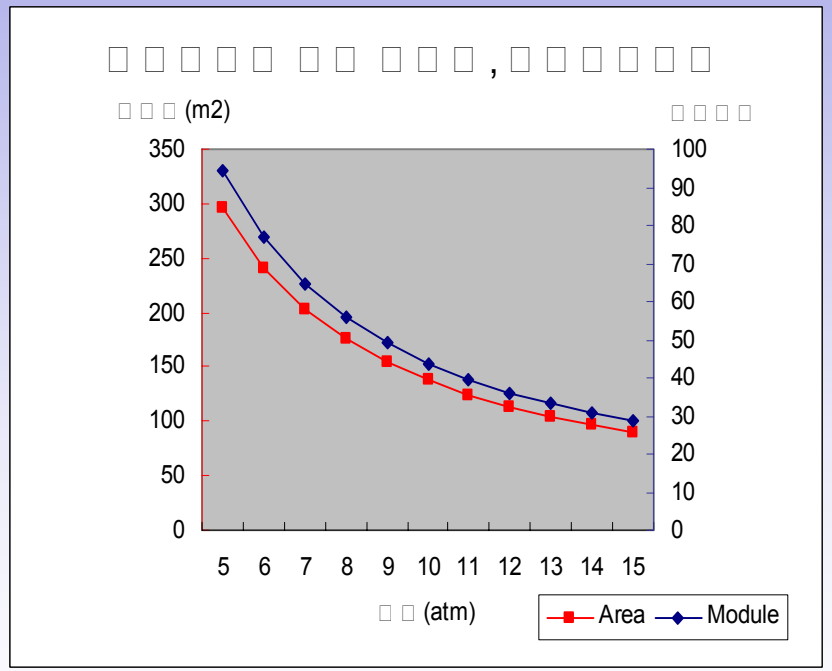
2) Fix selectivity as 20, then change permeability 20~100

3) Change permeability as well as selectivity 20~100

Simulation of 1 Membrane Module

1. Fix x_T as 0.01
   - Concentration and flow rate with pressure variation

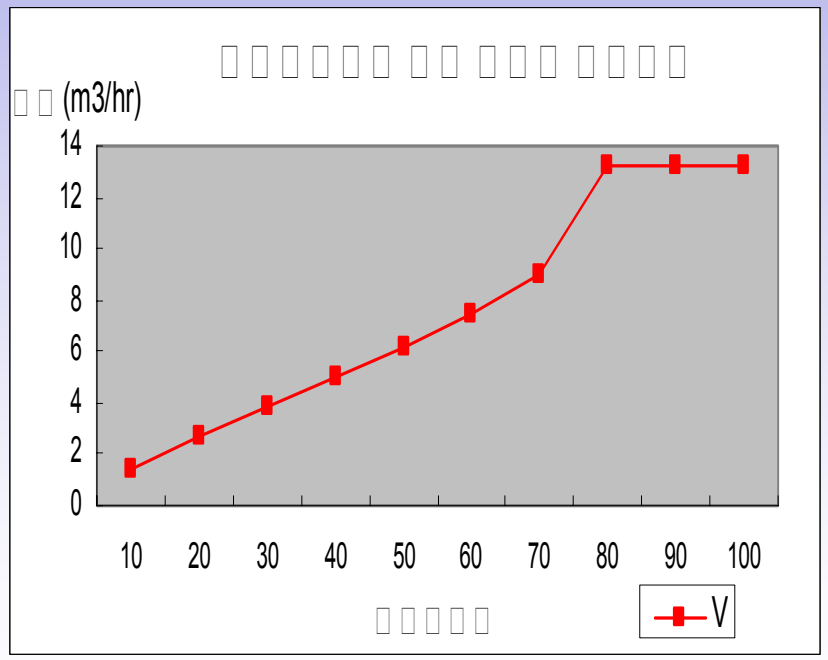


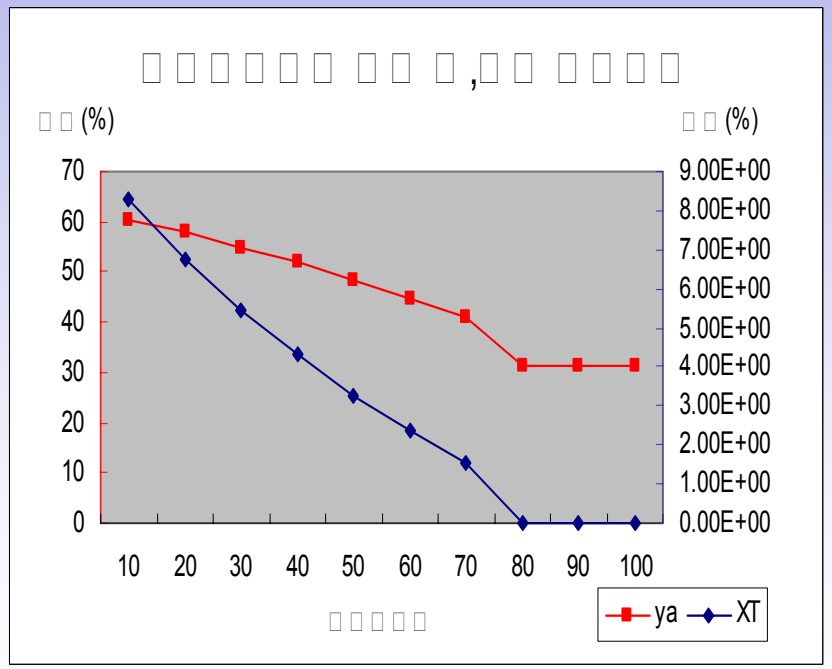


Simulation of 1 Membrane Module

2. Fix Pressure

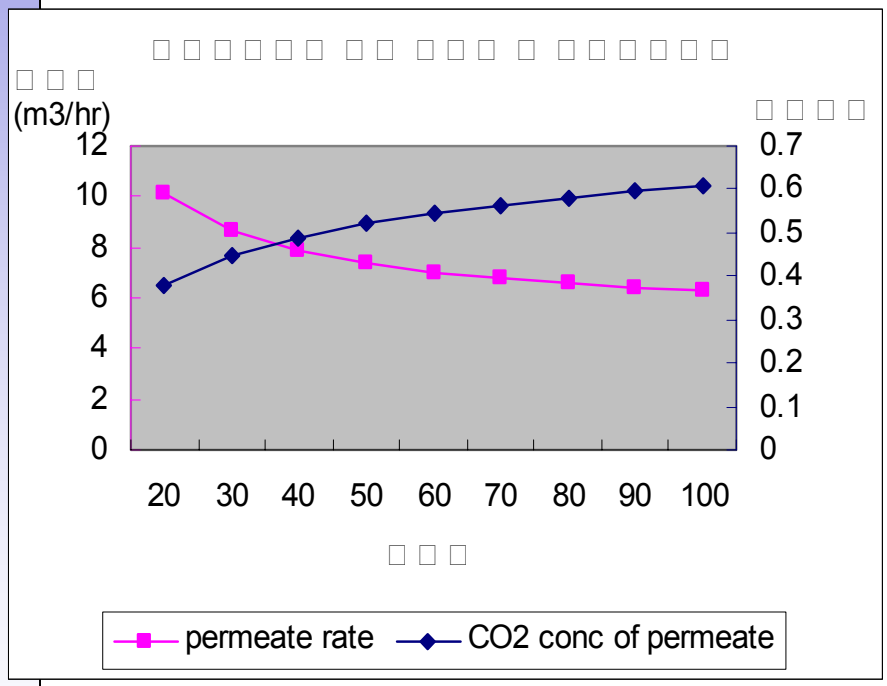
conc. and flow rate with variation of number of module

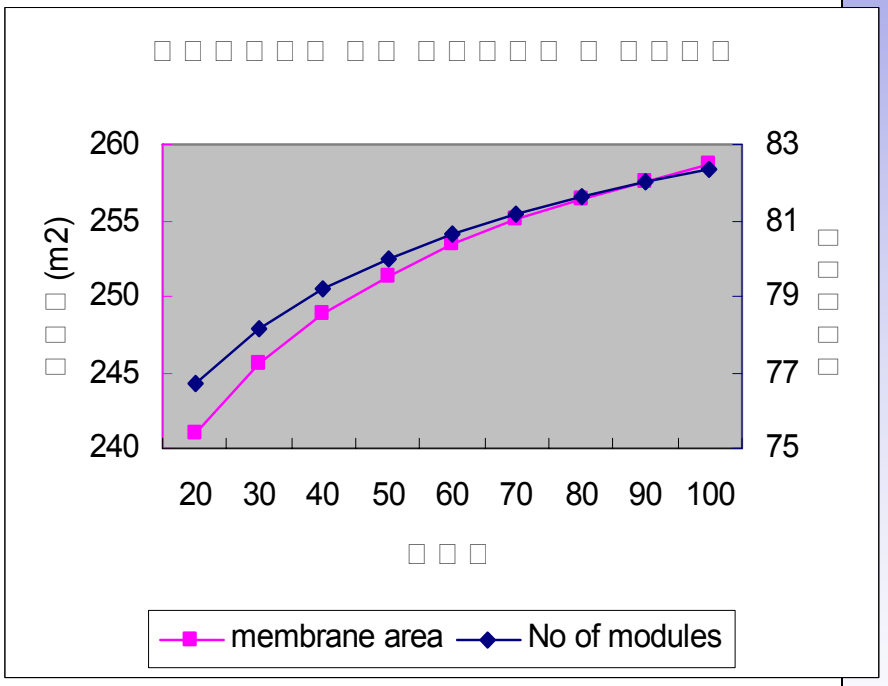




Simulation of 1 Membrane Module

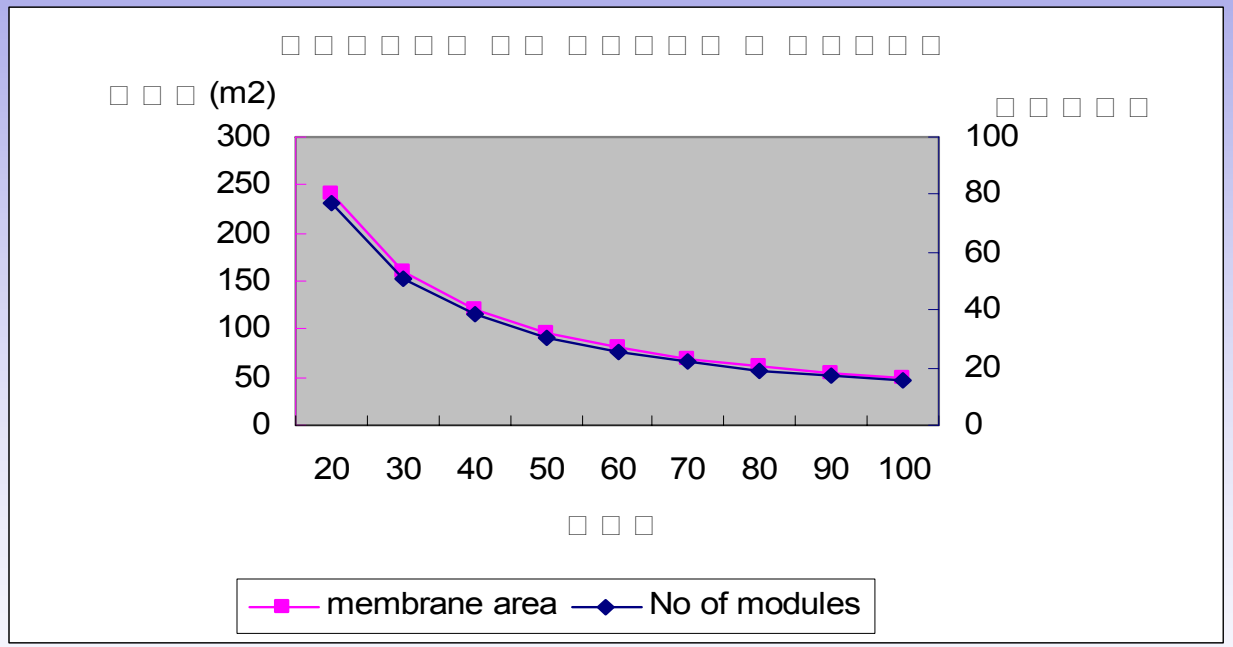
1. Permeability = 20, selectivity = 20~100





Simulation of 1 Membrane Module

2. Selectivity =20, permeability = 20~100



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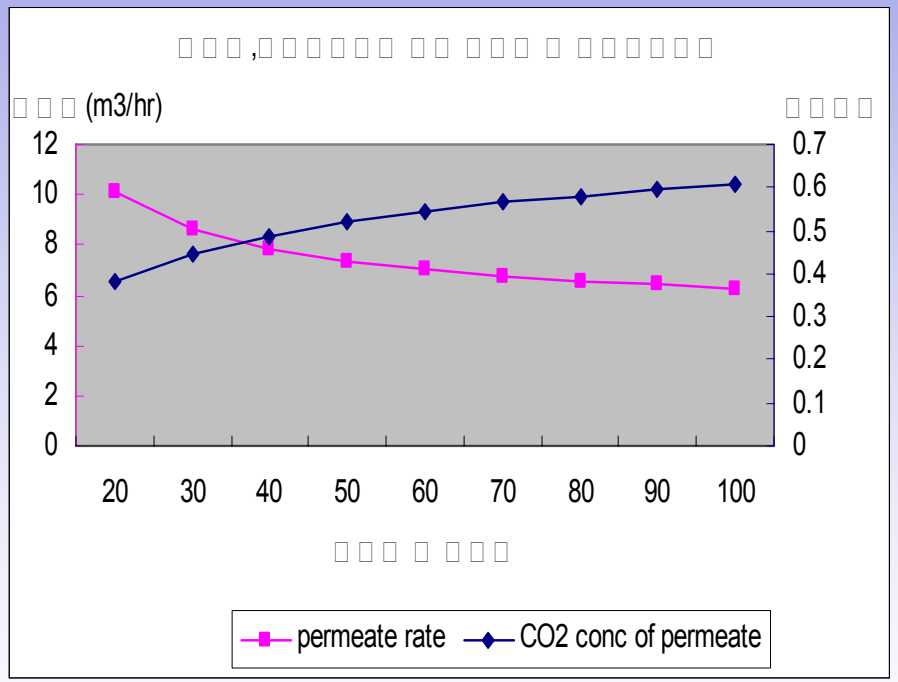
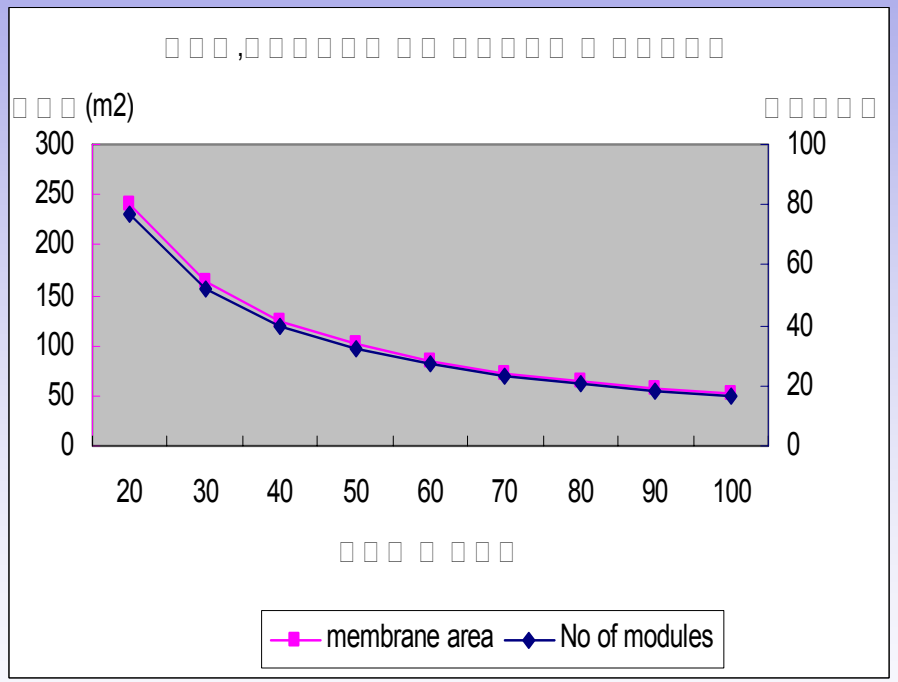
Simulation of 1 Membrane Module

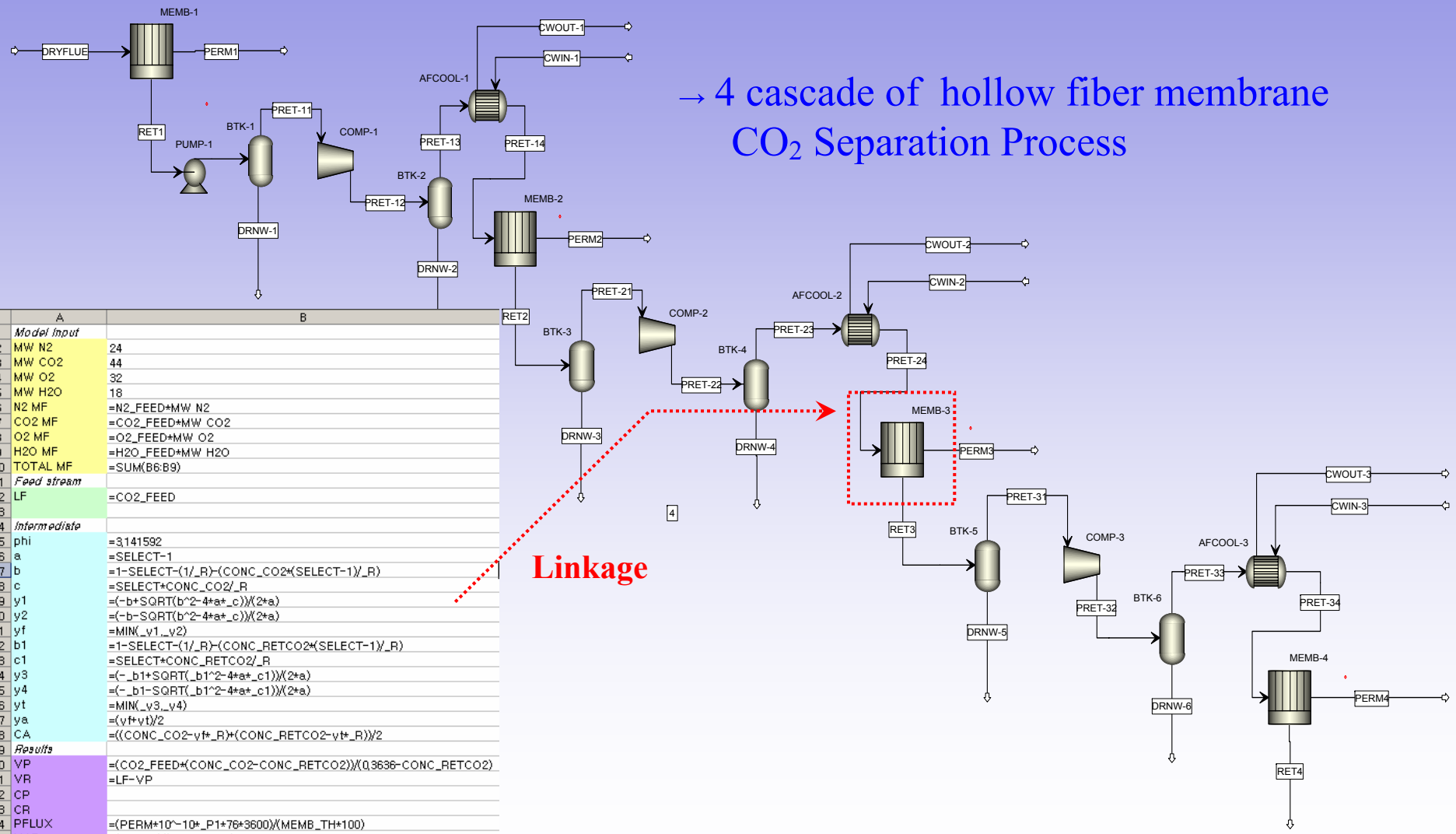
3. Permeability & selectivity = 20~100





Simulation of 4 membrane

- Simulation of CO_2 Separation Process by ASPEN (Excel) code (Peng-Rob equation)



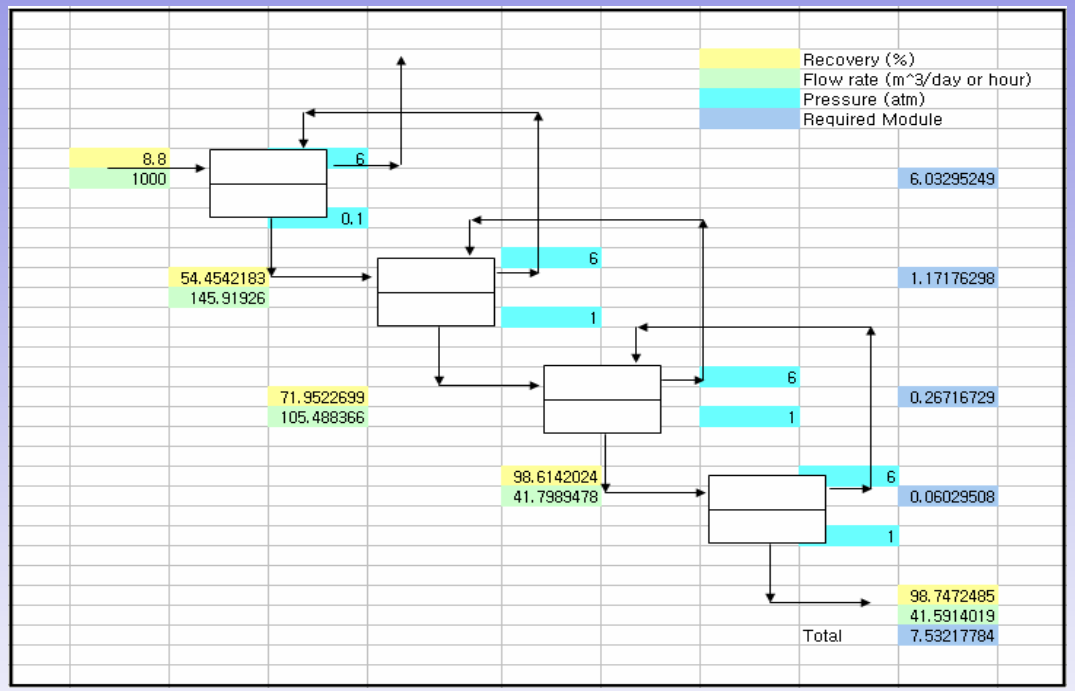
→ 4 cascade of hollow fiber membrane CO_2 Separation Process

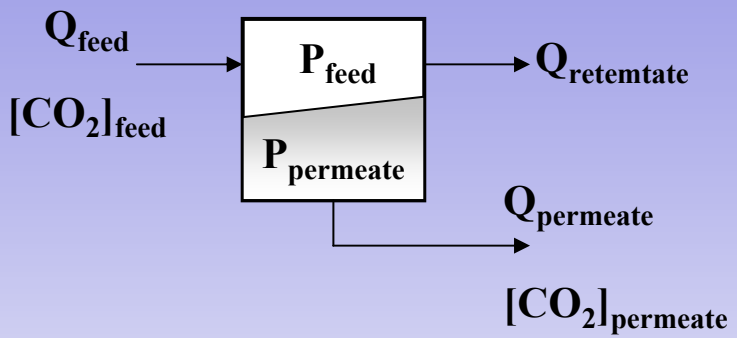
	A	B
1	*Model input*	
2	MW N2	24
3	MW CO2	44
4	MW O2	32
5	MW H2O	18
6	N2 MF	=N2_FEED*MW N2
7	CO2 MF	=CO2_FEED*MW CO2
8	O2 MF	=O2_FEED*MW O2
9	H2O MF	=H2O_FEED*MW H2O
10	TOTAL MF	=SUM(B6:B9)
11	*Feed stream*	
12	LF	=CO2_FEED
13		
14	*Intermediate*	
15	phi	=3.141592
16	a	=SELECT-1
17	b	=1-SELECT-(1/_R)-(CONC_CO2*(SELECT-1)/_R)
18	c	=SELECT*CONC_CO2/_R
19	y1	=(-b+SQRT(b^2-4*a*_c))/(2*a)
20	y2	=(-b-SQRT(b^2-4*a*_c))/(2*a)
21	yf	=MIN(_y1,_y2)
22	b1	=1-SELECT-(1/_R)-(CONC_RETCO2*(SELECT-1)/_R)
23	c1	=SELECT*CONC_RETCO2/_R
24	y3	=(-_b1+SQRT(_b1^2-4*a*_c1))/(2*a)
25	y4	=(-_b1-SQRT(_b1^2-4*a*_c1))/(2*a)
26	yt	=MIN(_y3,_y4)
27	ya	=(yf+yt)/2
28	CA	=((CONC_CO2-yf*_R)+(CONC_RETCO2-yt*_R))/2
29	*Results*	
30	VP	=(CO2_FEED*(CONC_CO2-CONC_RETCO2))/(0.3636-CONC_RETCO2)
31	VR	=LF-VP
32	CP	
33	CR	
34	PFLUX	=(PERM*10^-10*_P1*76*3600)/(MEMB_TH*100)
35	MAR	=(VP+va)/(PFLUX*CA)
36	EMAR	=(phi*MEMB_OD*MEMB_L)/10^3
37	MEMBAM	=MAR/EMAR
38	MODAM	=MEMBAM/NUM_HFM

User Model (Excel) for Membrane Modules in ASPEN code

Simulation of 4 membrane

- 4 cascade membrane modules without recycling retentate





- *Recovery, ψ (%)*

$$\psi(CO_2) = \frac{Q_{permeate} \times [CO_2]_{permeate}}{Q_{feed} \times [CO_2]_{feed}}$$

Stage	1	2	3	4	Total
Recovery (%)	54.45	71.95	98.61	98.74	-
Flow rate (m^3/day)	145.91	105.5	41.8	41.6	-
Required Module (EA)	6.03(. 7)	1.17(. 2)	0.27 (. 1)	0.06(1)	11

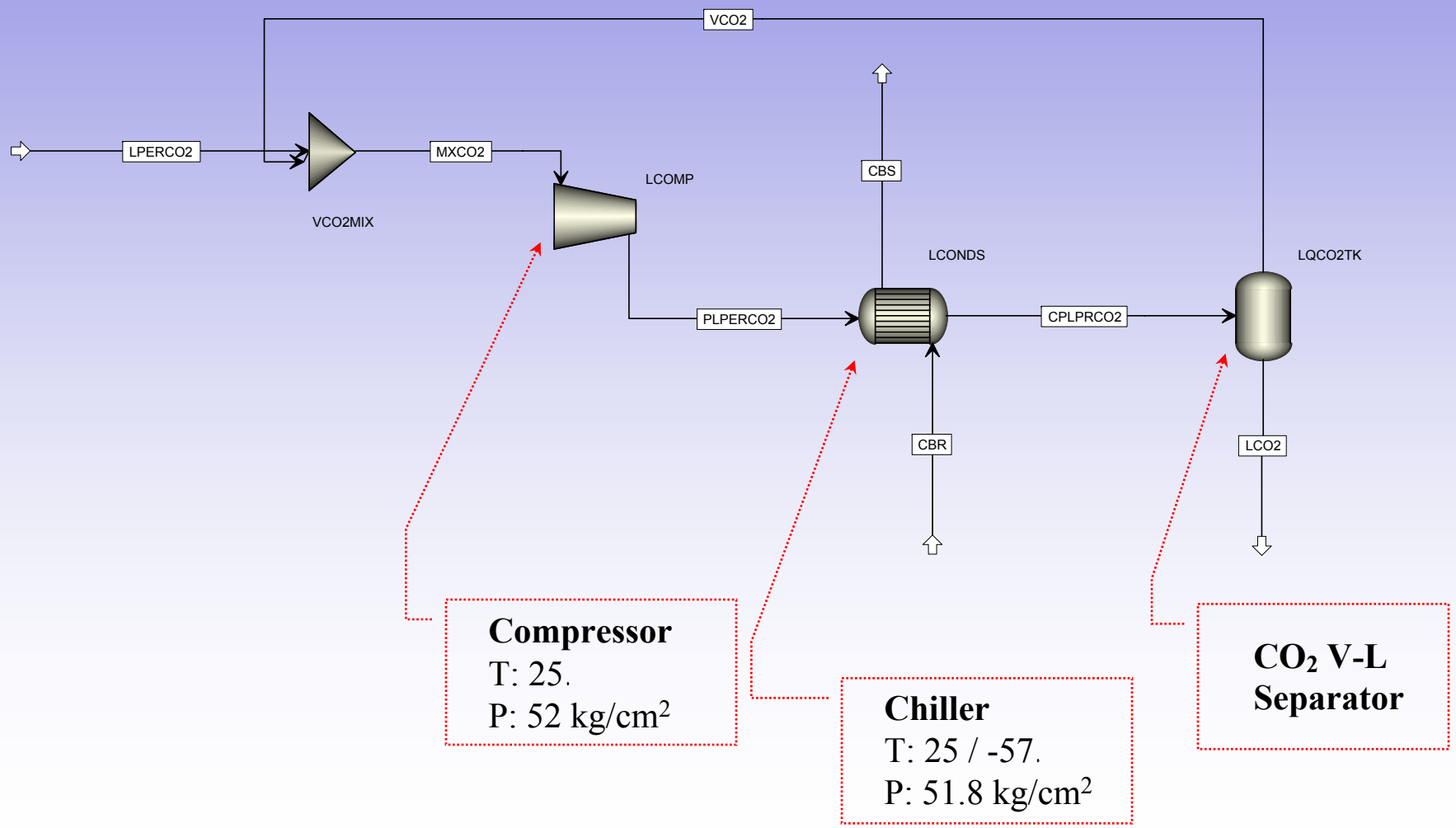
Simulation of 4 membrane

- 4 cascade membrane modules without recycling retentate

Operating Conditions		Comparison of result for Experiment/Simulation				
Parameter	Value (kg_f/cm^2)	Stage	Recovery (%)		Required amount of Module ($7m^2$)	
			SIM	EXP	SIM	EXP
P_{feed} / P_{perm}	6/0.1	1	54.45	51	7	8
	6/1	2	71.95	80	2	3
	6/1	3	98.61	94	1	1
	6/1	4	98.74	99.0	1	1(0.5)
P_{feed} / P_{perm}	6/1	1	25.67	32	40	20
	6/1	2	67.84	70	4	3
	6/1	3	94.40	89	1	2
	6/1	4	98.34	97	1	1

Simulation of CO2 Liquefaction Process

- Simulation of CO_2 Liquefaction Process by ASPEN code (Peng-Rob equation)



Conclusions

1. **Simulation method for CO2 membrane separation is developed**
   - Simulation program composed with H2O removal, membrane modules and CO2 liquefaction processes

2. **Evaluation of optimal condition of 1 membrane**
   - Obtaining optimum parameters with fixing the concentration of retreate and pressure as well as the variation of permeability and selectivity

3. **Development of membrane model using ASPEN & EXCEL**
   - Performing the simulation between ASPEN and EXCEL (User model)

Future Work

1. **Refine of membrane model using ASPEN & EXCEL**
   - **Link** between ASPEN and EXCEL (User model)

2. **Evaluation of optimum operation parameter**
   - Obtaining the optimum parameters with change of pressure, selectivity, permeability etc. with 4 membrane module

3. **Simulation for detail equipments**
   - Energy requirement calculations for Vacuum pump, Compressor, Condenser for CO_2 liquefaction process

4. **Energy requirement & cost calculations through exergy analysis**
   - Using each stream results by simulation for exergy calculation

Thank you