

천연가스로부터 개질반응 및 PSA에 의한 고순도 수소 생산

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조정호

목 차

- 1 조정호 교수 및 화학공정연구실 연구실 소개
- 2 Reforming과 WGS반응에 대한 수소 제조 Kinetic Parameters 결정
- 3 천연가스 원료 및 공정모사 조건
- 4 이성분계에 실험데이터로부터 BIP를 선정하는 과정
- 5 천연가스 원료별 전산모사 결과

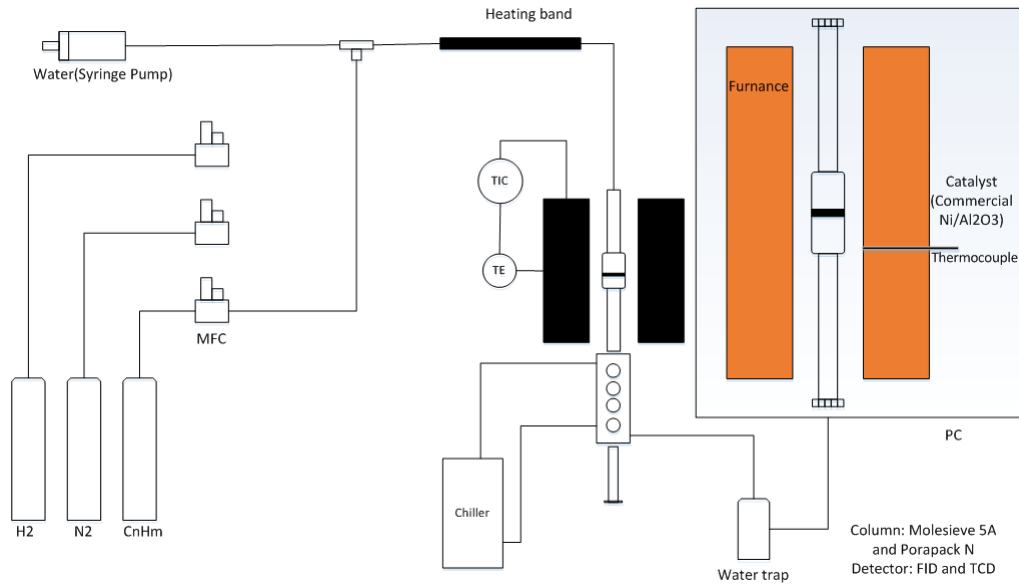
상용 촉매 별 천연가스 개질 반응 Kinetic Data 수집:

▶ 촉매의 재질 및 크기:

- 재질: Reformer 촉매 Ni/ α -Al₂O₃,
- Pellet Size: (1) 8x8x3 mm, (2) 6x6 mm



실험 장치에 대한 모식도 및 사진



Steam Reforming 반응실험:

➤ Steam Reforming에 대한 반응실험:

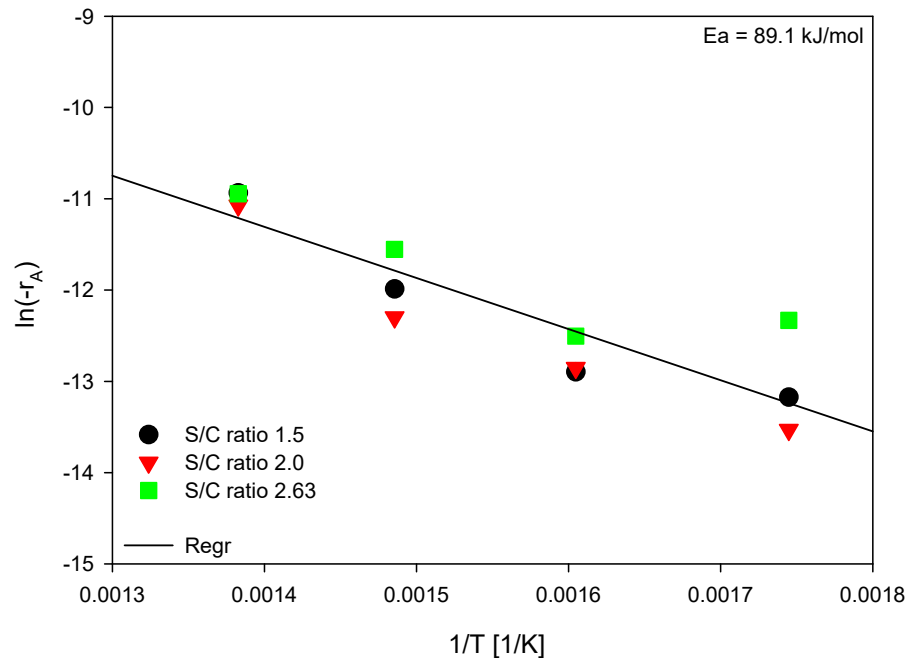
Items	Conditions
Catalyst	Ni/ α -Al ₂ O ₃
Temperature [°C]	350, 400, 450
Steam Carbon Ratio	Steam/Carbon Ratio: 1.50 Steam/Carbon Ratio: 2.00 Steam/Carbon Ratio: 2.63
Constant concentration of H ₂ O	N ₂ (80) : C _n H _m (20) N ₂ (85) : C _n H _m (15) N ₂ (90) : C _n H _m (10)

개질 실험 결과:

➤ 순수한 가스의 Steam Reforming 반응: Power Rate Law Model

- Methane:
- Activation Energy, E_a

$$-r' = k_0 \text{EXP}(-E_a/RT) [P_{\text{CH}_4}]^\alpha [P_{\text{H}_2\text{O}}]^\beta \xrightarrow{\text{양변 자연로그}} \ln(-r') = \ln(k_0 [P_{\text{CH}_4}]^\alpha [P_{\text{H}_2\text{O}}]^\beta) - (E_a/R)(1/T)$$



➡ E_a (Methane, Ni catalyst) = 89.1 kJ/mol

개질 실험 결과:

➤ 순수한 가스의 Steam Reforming 반응: Power Rate Law Model

- Methane:
- Reaction Order, α , β

STEP 1.

$$\ln(-r') = \ln(k_0) - (E_a/R)(1/T) + \alpha \ln(P_{CH_4}) + \beta \ln(P_{H_2O})$$

충분한 농도

Plotting

STEP 2.

$$\ln(-r') = \ln(k_0) - (E_a/R)(1/T) + \alpha \ln(P_{CH_4}) + \beta \ln(P_{H_2O})$$

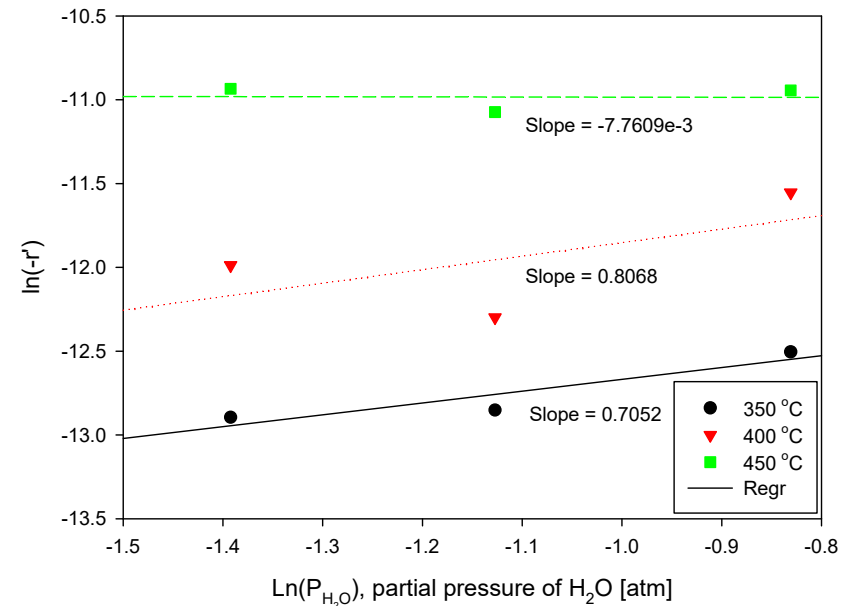
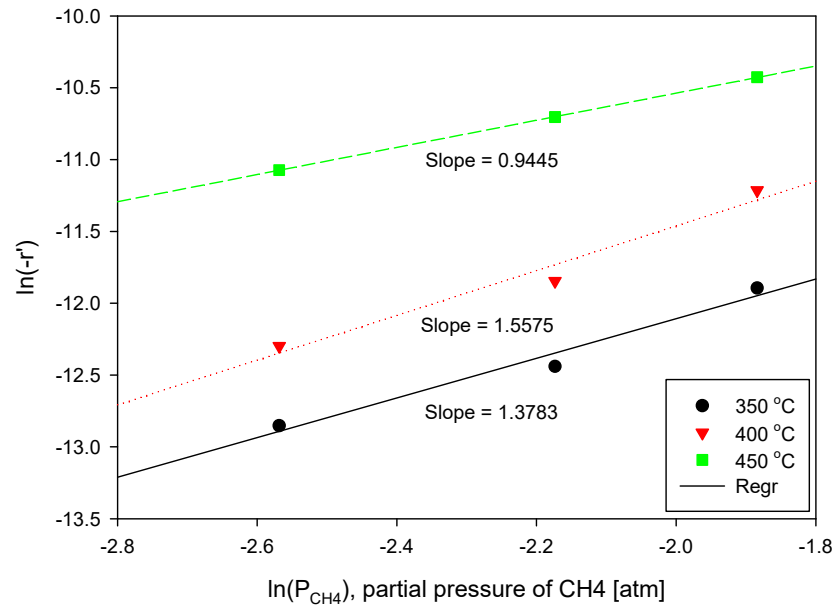
충분한 농도

Plotting

개질 실험 결과:

➤ 순수한 가스의 Steam Reforming 반응: Power Rate Law Model

- Methane:
- Reaction Order, α , β



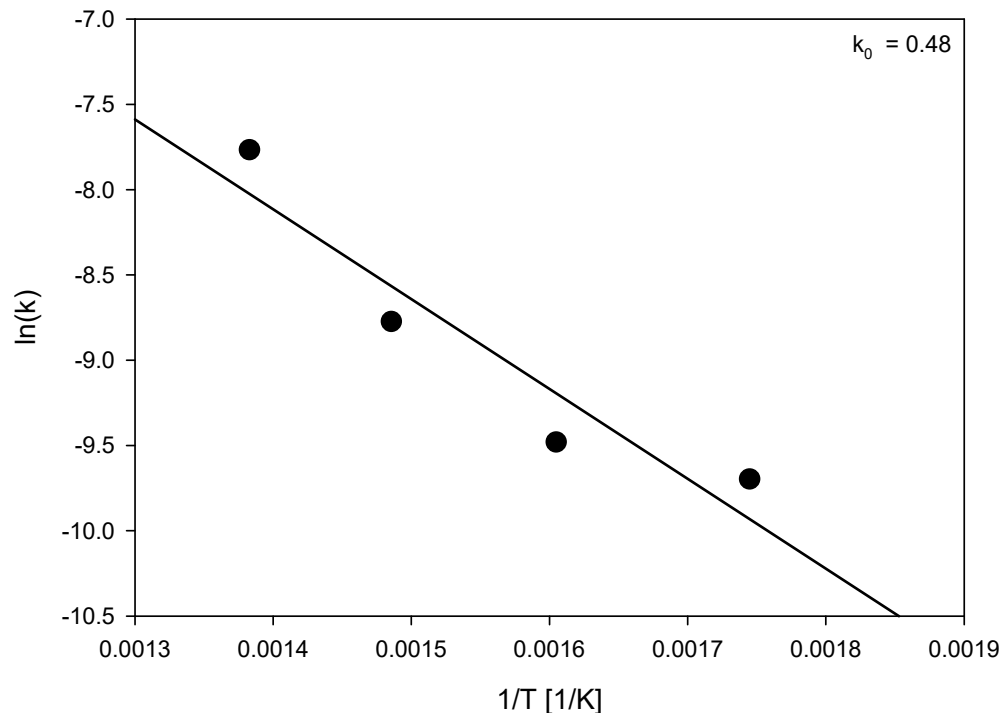
➡ α (Methane)=1.3, β (Methane) = 0.5

개질 실험 결과:

➤ 순수한 가스의 Steam Reforming 반응: Power Rate Law Model

- Methane:
- Pre-exponential Factor, k_0

$$k = k_0 \exp(-E_a/RT) \xrightarrow{\text{양변 자연로그}} \ln(k) = \ln(k_0) - (E_a/R)(1/T)$$



$$k_0 (\text{Ni}/\alpha\text{-Al}_2\text{O}_3 \text{ catalyst}) = 0.48$$

개질 실험 결과:

➤ 순수한 탄화수소 가스의 Steam Reforming 반응 속도식:

$$-r' = k_0 \text{EXP}(-E_a/RT) [P_{\text{HC}}]^\alpha [P_{\text{H}_2\text{O}}]^\beta$$

Component	k_0	E_a (kJ/gmol)	α	β
CH ₄	0.48	89.1	1.3	0.5
C ₂ H ₆	67.63	43.8	-0.6	1.5
C ₃ H ₈	17.20	77.8	0.9	-0.8
C ₄ H ₁₀	0.79	1.80	1.0	0.0

개질 실험 결과: Langmuir-Hinshelwood Model

➤ 순수한 탄화수소 가스의 Steam Reforming 반응:

$$-r = \frac{k_s K_A K_B P_{C_nH_m} P_{H_2O}}{(1 + K_A P_{C_nH_m} + K_B P_{H_2O})^2}$$

k_s = 표면반응 속도상수

K_A = C_nH_m 의 흡착 평형상수

K_B = H_2O 의 흡착 평형상수

$P_{C_nH_m}$, P_{H_2O} = 반응물의 농도



실험 data,
Polymath program - Nonlinear regression을 이용

개질 실험 결과: Langmuir-Hinshelwood Model

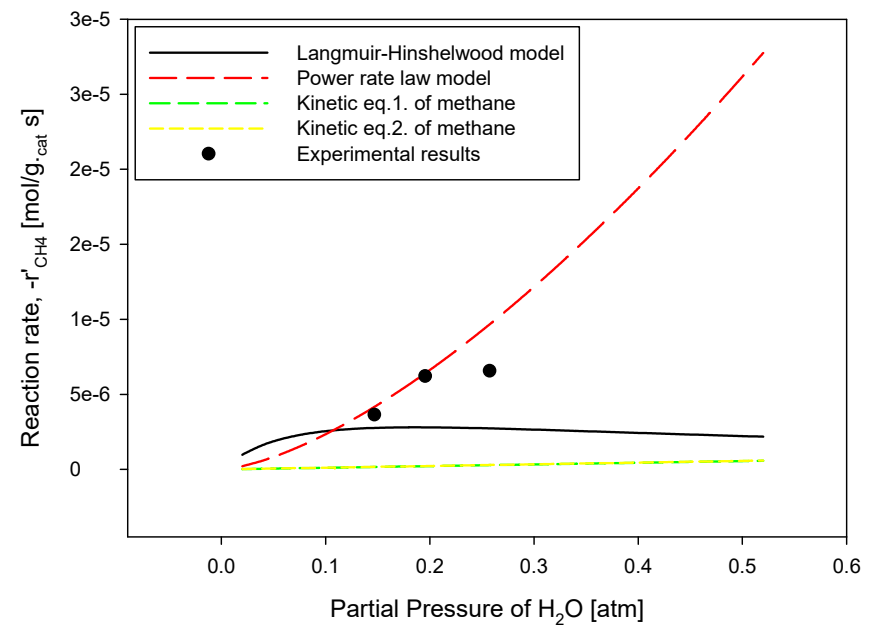
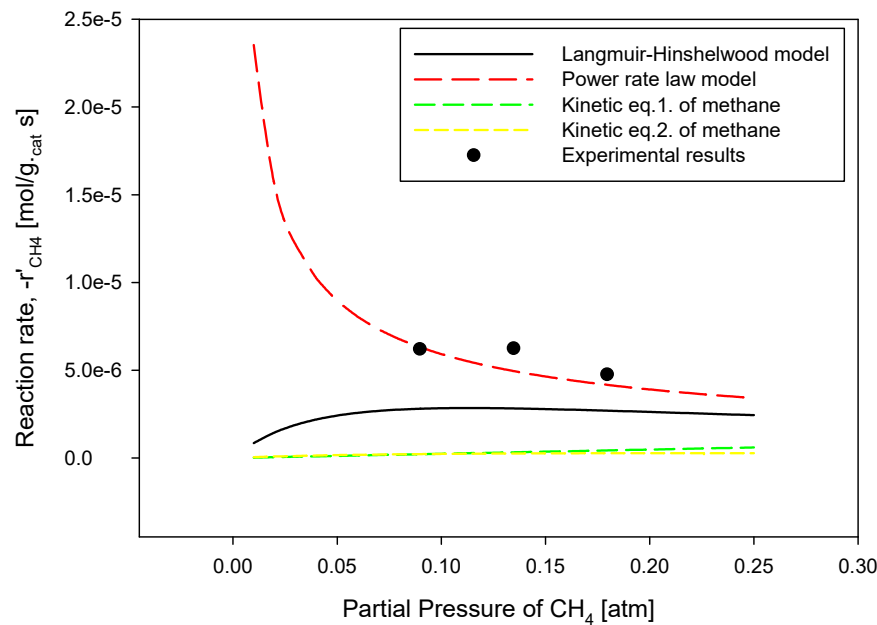
➤ Parameters for Langmuir-Hinshelwood Kinetic Model:

Gas	Temperature (°C)	k_s	K_A	K_B
Methane	350	4.66E-06	102.00	60.08
	400	1.20E-05	102.00	71.68
	450	2.72E-05	102.00	66.44
Ethane	350	2.89E-05	102.00	101.50
	400	4.52E-05	21.05	21.63
	450	6.66E-05	49.16	7.125
Propane	350	6.28E-07	102.00	24.60
	400	3.32E-06	102.00	17.0146
	450	1.39E-05	102.00	21.88
Butane	350	0.000379	7.40	9.29
	400	0.000391	7.14	8.87
	450	0.000401	7.75	9.48

개질 실험 결과: Langmuir-Hinshelwood Model

➤ Power Rate Law Model vs. Langmuir-Hinshelwood Kinetic Model:

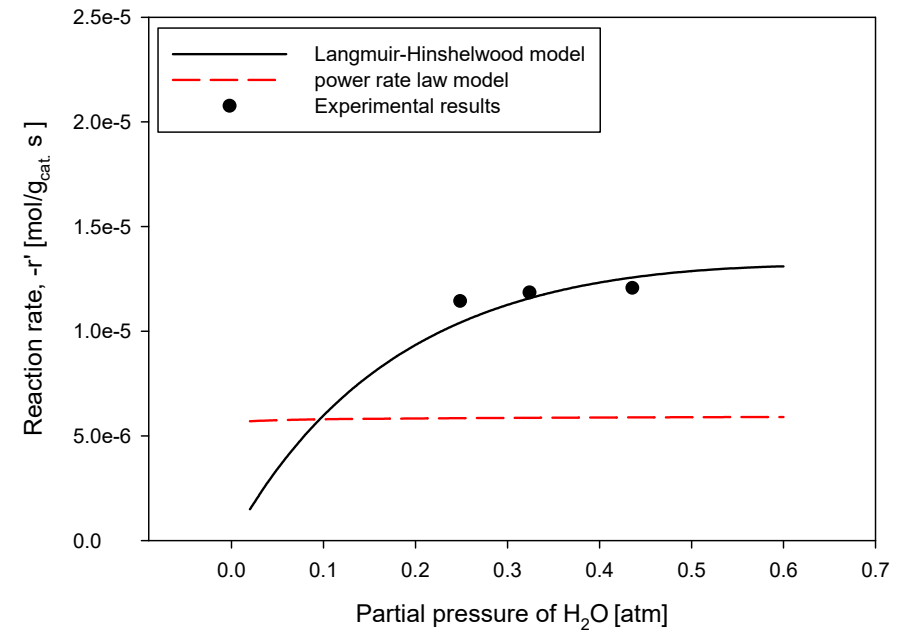
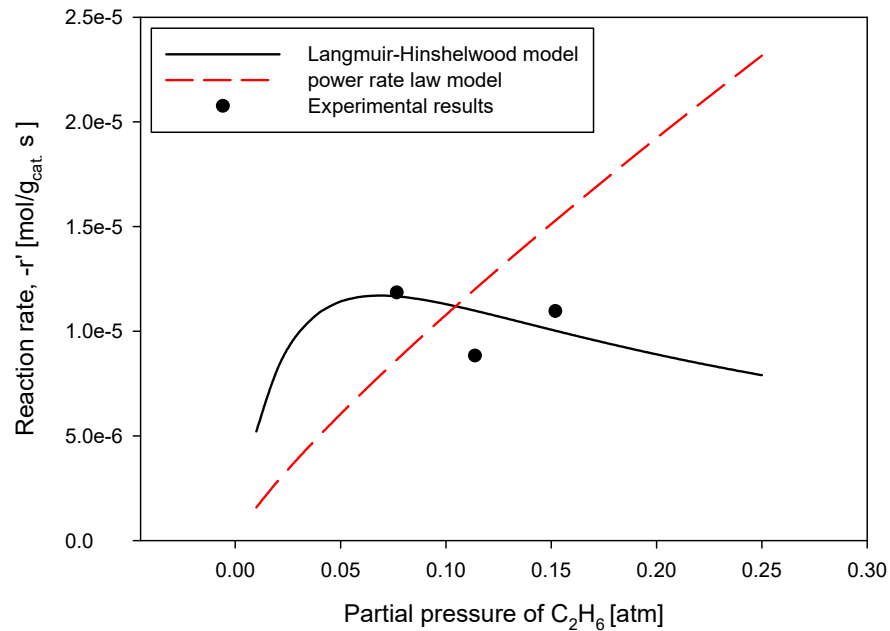
- Methane:



개질 실험 결과: Langmuir-Hinshelwood Model

➤ Power Rate Law Model vs. Langmuir-Hinshelwood Kinetic Model:

- Ethane:



Water Gas Shift 반응에 대한 Kinetic Model:

➤ CO의 Water Gas Shift 반응 속도식:

$$-r'_{\text{CO}} = 8.42 \times 10^{-5} \text{EXP}(-14.8 \times 10^3 / RT) [C_{\text{CO}}]^{0.0} [C_{\text{H}_2\text{O}}]^{-0.2}$$

전산모사를 위해 적용한 Kinetic Data

➤ Reformer에 대한 반응식 선정 및 실험 데이터로부터 Kinetic parameters 적용

			k_0	Ea [kJ/mol]	Reaction order	
					α	β
CH ₄	Langmuir-Hinshelwood Equation	$-r_{\text{CH}_4} = \frac{k_1 K_{\text{CH}_4} K_{\text{H}_2\text{O}} P_{\text{CH}_4} P_{\text{H}_2\text{O}}}{SS^2}$	5,294.6	96.6313	0.9	0.7
	Reaction stoichiometry	$\text{CH}_4 + \text{H}_2\text{O} \xrightarrow{k_1} \text{CO} + 3\text{H}_2$				
C ₂ H ₆	Langmuir-Hinshelwood Equation	$-r_{\text{C}_2\text{H}_6} = \frac{k_2 K_{\text{C}_2\text{H}_6} K_{\text{H}_2\text{O}} P_{\text{C}_2\text{H}_6} P_{\text{H}_2\text{O}}}{SS^2}$	14,569	79.4830	0.7	-0.7
	Reaction stoichiometry	$\text{C}_2\text{H}_6 + 2\text{H}_2\text{O} \xrightarrow{k_2} 2\text{CO} + 5\text{H}_2$				

전산모사를 위해 적용한 Kinetic Data

➤ Reformer에 대한 반응식 선정 및 실험 데이터로부터 Kinetic parameters 적용

			k_0	Ea [kJ/mol]	Reaction order	
					α	β
C_3H_8	Langmuir-Hinshelwood Equation	$-r_{C_3H_8} = \frac{k_3 K_{C_3H_8} K_{H_2O} P_{C_3H_8} P_{H_2O}}{SS^2}$	99.715	39.136	1.0	-0.8
	Reaction stoichiometry	$C_3H_8 + 3H_2O \xrightarrow{k_3} 3CO + 7H_2$				
nC_4H_{10}	Langmuir-Hinshelwood Equation	$-r_{C_4H_{10}} = \frac{k_4 K_{C_4H_{10}} K_{H_2O} P_{C_4H_{10}} P_{H_2O}}{SS^2}$	342.23	28.54	1.0	0.2
	Reaction stoichiometry	$C_4H_{10} + 4H_2O \xrightarrow{k_2} 4CO + 9H_2$				

$$SS = 1 + K_{CH_4} P_{CH_4} + K_{C_2H_6} P_{C_2H_6} + K_{C_3H_8} P_{C_3H_8} + K_{C_4H_{10}} P_{C_4H_{10}} + K_{H_2O} P_{H_2O}$$

K_{C_1}	K_{H_2O}	K_{C_2}	K_{C_3}	K_{C_4}
2.397589	3.48303	0.135456	1.116676	0.119309

Natural Gas Feed Composition by KOGAS

Stream No.	1	2	3	4	5	6	7
Case	Lean	Rich	Max N ₂	Typical 1	Typical 2	최저	순수메탄
Nitrogen	0.00	0.00	1.00	0.20	0.2	0.19	0
Methane	96.74	85.12	94.33	91.31	93.08	96.65	100
Ethane	1.89	8.63	1.97	5.47	4.49	0.58	0
Propane	0.68	4.14	2.50	2.06	1.53	0.08	0
i-Butane	0.34	1.10	0.10	0.45	0.33	0.11	0
N-Butane	0.34	0.90	0.10	0.48	0.36	0	0
i-Pentane	0.01	0.10	0.00	0.02	0.02	0	0
N-Pentane	0.00	0.01	0.00	0.00	0.00	0	0
MW	16.7904	19.3180	17.2243	17.8146	17.4272	16.2198	16.0428
GHV	9,875	11,154	9,940	10,363	10,167	9,557	9,497
LHV	8,904	10,097	8,967	9,360	9,177	8,607	8,551

Gas volume계산에 사용된 Standard Condition →

Standard Conditions:

Standard Temperature: C

Standard Pressure: kg/cm²

Use Std. Pressure and Temperature to Calculate Std. Vapor Volume

Standard Vapor Volume: m³/kg-mol

보령LNG터미널에서 취급하는 LNG의 조성:

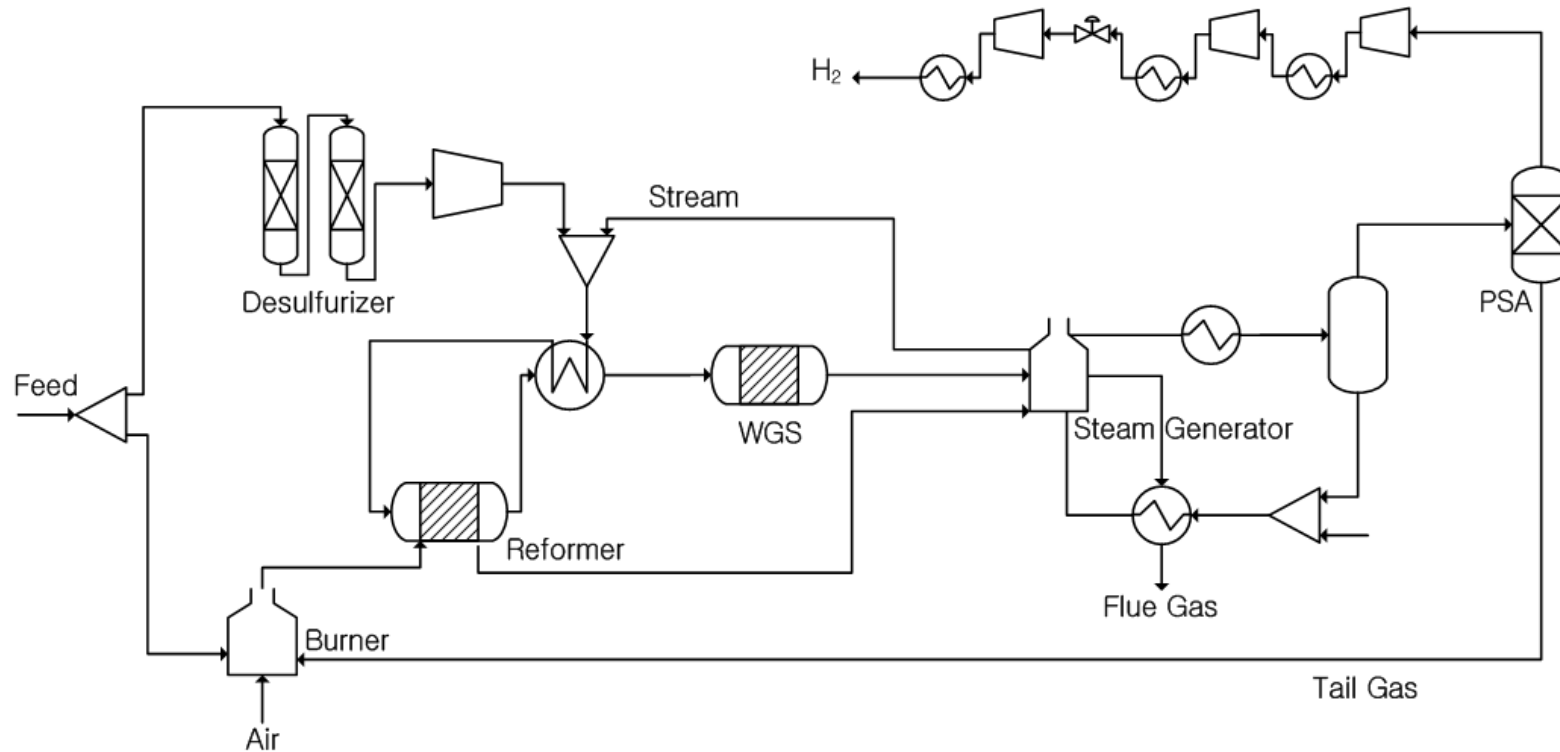
Component	Composition (Mol%)		
	Case 1 (Lean)	Case 2 (Typical)	Case 3 (Rich)
Nitrogen	0.2	0.19	0.00
Methane	97.70	96.74	85.12
Ethane	2.10	2.35	8.63
Propane	-	0.50	4.14
i-Butane	-	0.09	1.10
n-Butane	-	0.11	0.90
i-Pentane	-	0.02	0.10
n-Pentane	-	-	0.01
Molecular weight	16.36	16.63	19.32
Gross heating value, @ 0 °C & 1 atm(kcal/Nm ³)	9,631	9,768	11,195
SG of liquid	0.425	0.430	0.478
Gas compressibility factor @ 0 °C & 1 atm	0.9969	0.9968	0.9957
Gas density (real) @ 0 °C & 1atm (kg/Nm ³)	0.7322	0.7444	0.8656

KOGAS와
동일

* Nm³ 은 0°C, 1 atm 에서 측정

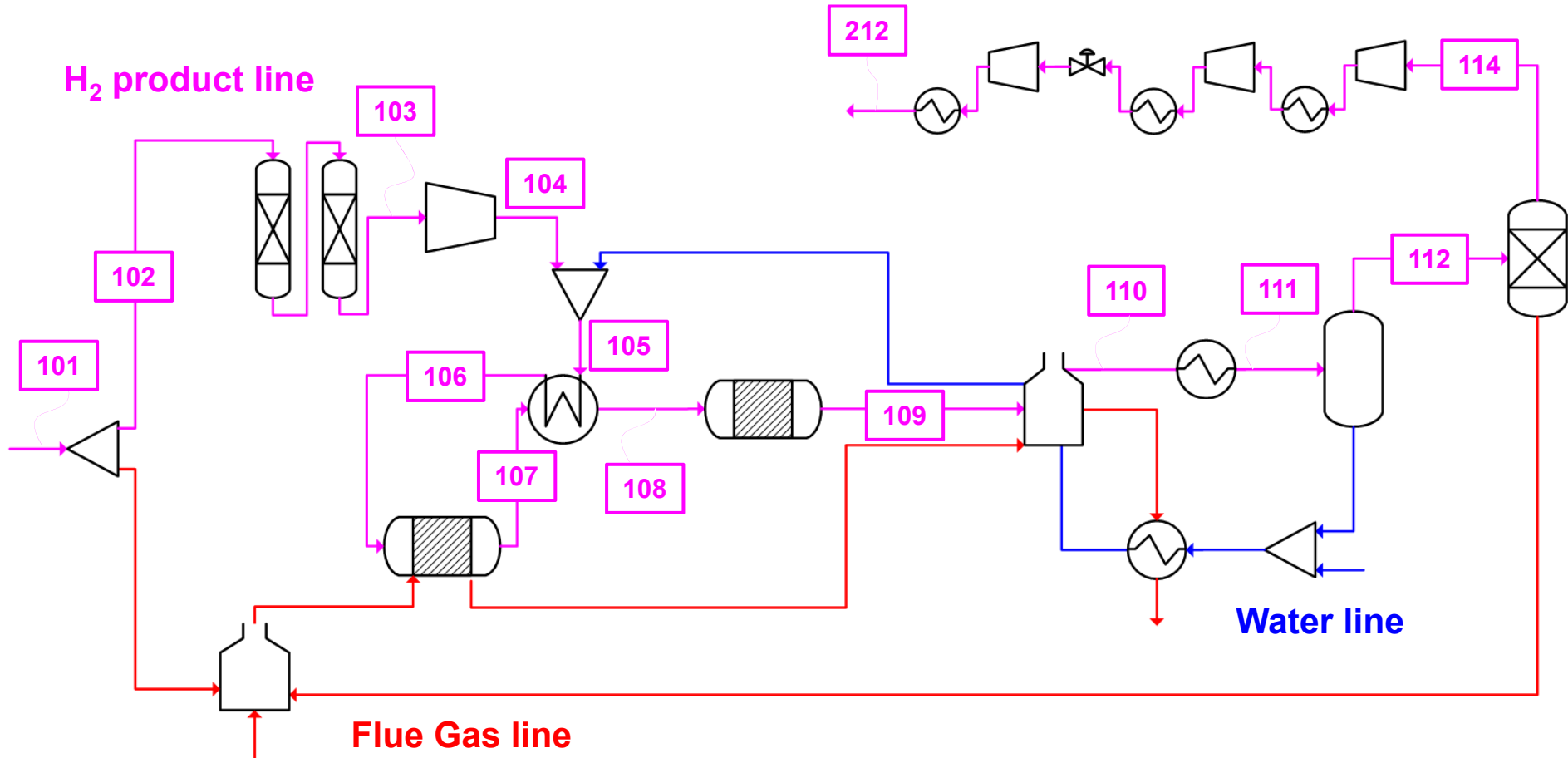
Process Flow Sheet for Reforming System:

천연가스를 통해 500 kg/day 수소를 생산하는 수소생산 공정의 공정도



Process Flow Sheet for Reforming System:

수소 생산 공정은 크게 3개의 라인(**H₂ product line**, **Flue Gas line**, **Water line**)으로 나누어짐.



전산모사 조건

운전 변수	운전 조건
NG Feed Gas Flow	수소 농도 99.999 vol.% 이상, 용량은 500 kg/day 이상을 생산하기 위한 천연가스 원료유량
NG gas GHV	10,200 Kcal/Nm ³
S/C ratio	3.0
H ₂ production rate	500 kg/day
H ₂ purity	99.999%
H ₂ recovery at PSA	80.0%
H ₂ O content in PSA feed	0.7mole%
Feed Gas Pressure	4.0 bar
Excess Air %	10%

열역학 모델식 및 매개변수 선정:

➤ Soave-Redlich-Kwong Equation 사용

$$P = \frac{RT}{v - b} - \frac{a(T_c) \cdot \alpha(T_r, \omega)}{v(v + b)}$$

- a와 b는 각각 energy parameter와 size parameter

$$a = 0.42747 \frac{R^2 T_c^2}{P_c} \quad ; \quad b = 0.08664 \frac{RT_c}{P_c}$$

- α 는 alpha function으로 편심인자와 환산온도의 함수

$$\alpha_i(T) = \left[1 + m_i \left(1 - T_{ri}^{1/2} \right) \right]^2$$

$$m_i = 0.48508 + 1.55171\omega_i - 0.15613\omega_i^2$$

열역학 모델식 및 매개변수 선정:

- 본 공정과 같이 수소를 다량으로 함유하고 있고, 고온 공정인 경우에는 Original alpha function 은 실제와는 다른 상 거동을 나타내며 많은 오차를 발생시키므로, Twu 등이 제안한 다른 형태의 alpha function을 사용함.

$$\alpha = T_r^{C_3(C_2-1)} \exp[C_1(1 - T_r^{C_2C_3})]$$

■ 성분에 대한 alpha Function에 대한 계수들

Component	C ₁	C ₂	C ₃
CH ₄	0.5143	0.9902	1.0000
H ₂ O	0.3569	0.8743	2.4806
C ₂ H ₆	0.2423	0.8800	1.9844
C ₃ H ₈	0.2348	0.8661	2.2075
NC ₄	0.1847	0.8746	2.9481
CO	0.2079	0.8606	1.7188
H ₂	1.2528	13.2690	0.0400
CO ₂	1.2344	1.3267	0.6498
N ₂	0.1522	0.8944	2.3403
O ₂	0.1535	0.9088	2.4355

열역학 모델식 및 매개변수 선정:

The mixing rules available for the SRK EOS state are shown below,

$$a_{mix} = \sum_{i=1}^N \sum_{j=1}^N x_i x_j a_{ij} \quad b_{mix} = \sum_{i=1}^N b_i x_i$$

$$a_{ij} = \sqrt{a_i a_j} (1 - k_{ij})$$

Regressed binary interaction parameter

SRK INTERACTION PARAMETERS

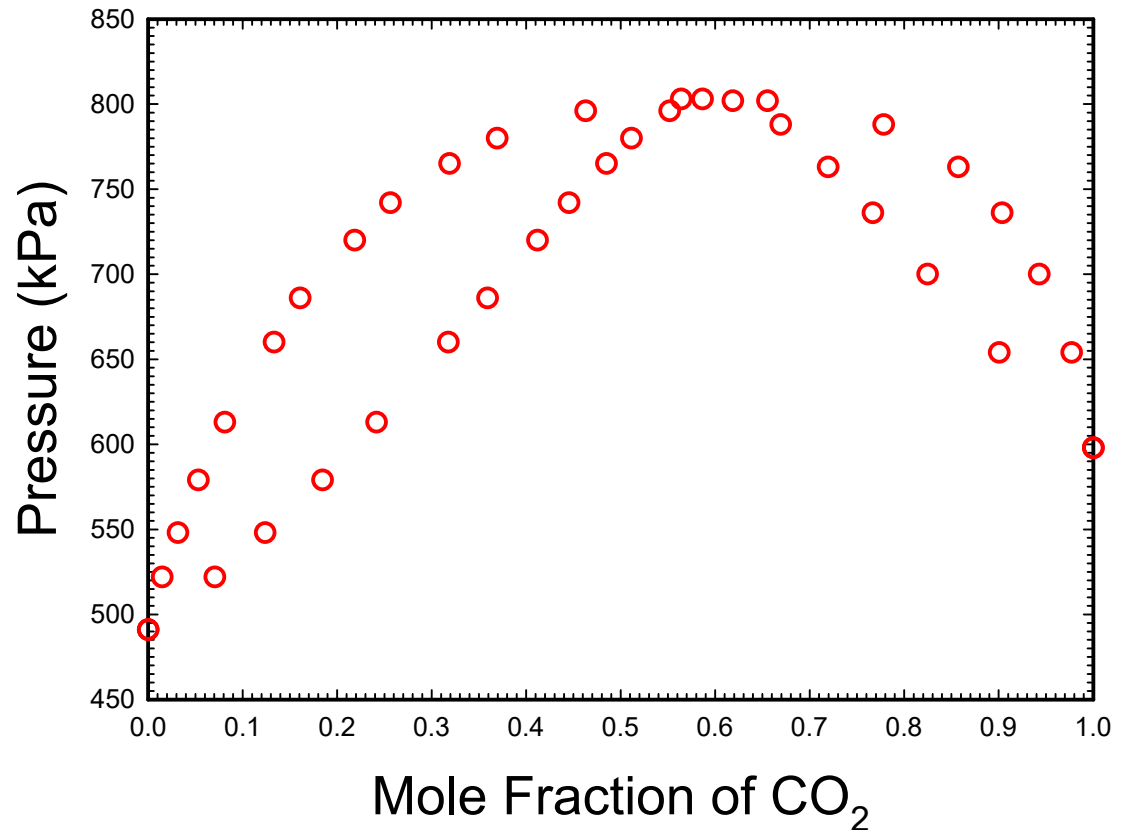
$$K_{IJ} = A(I,J) + B(I,J)/T + C(I,J)/T^{**2} + D(I,J)*T$$

I	J	KA(I,J)	KB(I,J)	KC(I,J)	KD(I,J)	UNITS	FROM
1	2	0.5200	0.00	0.00	0.00	DEG K	SIMSCI BANK
1	3	-7.800E-03	0.00	0.00	0.00	DEG K	SIMSCI BANK
1	4	9.000E-03	0.00	0.00	0.00	DEG K	SIMSCI BANK
1	5	5.600E-03	0.00	0.00	0.00	DEG K	SIMSCI BANK
1	6	0.0322	0.00	0.00	0.00	DEG K	SIMSCI BANK
1	7	-0.0200	0.00	0.00	0.00	DEG K	SIMSCI BANK
1	8	0.0933	0.00	0.00	0.00	DEG K	SIMSCI BANK
1	9	0.0300	0.00	0.00	0.00	DEG K	SIMSCI BANK
1	10	0.0600	0.00	0.00	0.00	DEG K	MW CORRELATION
2	3	0.5500	0.00	0.00	0.00	DEG K	SIMSCI BANK
2	4	0.5300	0.00	0.00	0.00	DEG K	SIMSCI BANK
2	5	0.5200	0.00	0.00	0.00	DEG K	SIMSCI BANK
2	6	0.2000	0.00	0.00	0.00	DEG K	SIMSCI BANK
2	7	0.4000	0.00	0.00	0.00	DEG K	SIMSCI BANK
2	8	0.2300	0.00	0.00	0.00	DEG K	SIMSCI BANK
2	9	0.5300	0.00	0.00	0.00	DEG K	SIMSCI BANK
3	4	-2.200E-03	0.00	0.00	0.00	DEG K	SIMSCI BANK
3	5	6.700E-03	0.00	0.00	0.00	DEG K	SIMSCI BANK
3	6	0.0200	0.00	0.00	0.00	DEG K	SIMSCI BANK
3	7	-0.0100	0.00	0.00	0.00	DEG K	SIMSCI BANK
3	8	0.1363	0.00	0.00	0.00	DEG K	SIMSCI BANK
3	9	0.0600	0.00	0.00	0.00	DEG K	SIMSCI BANK
3	10	0.0600	0.00	0.00	0.00	DEG K	MW CORRELATION
4	5	0.0000	0.00	0.00	0.00	DEG K	SIMSCI BANK
4	6	0.0200	0.00	0.00	0.00	DEG K	SIMSCI BANK
4	7	0.1000	0.00	0.00	0.00	DEG K	SIMSCI BANK
4	8	0.1289	0.00	0.00	0.00	DEG K	SIMSCI BANK
4	9	0.0900	0.00	0.00	0.00	DEG K	SIMSCI BANK
4	10	0.0900	0.00	0.00	0.00	DEG K	MW CORRELATION
5	6	0.0300	0.00	0.00	0.00	DEG K	SIMSCI BANK
5	7	-0.5100	0.00	0.00	0.00	DEG K	SIMSCI BANK
5	8	0.1430	0.00	0.00	0.00	DEG K	SIMSCI BANK
5	9	0.1130	0.00	0.00	0.00	DEG K	SIMSCI BANK
5	10	0.1130	0.00	0.00	0.00	DEG K	MW CORRELATION
6	7	0.0400	0.00	0.00	0.00	DEG K	SIMSCI BANK
6	8	0.0500	0.00	0.00	0.00	DEG K	SIMSCI BANK
6	9	0.0400	0.00	0.00	0.00	DEG K	SIMSCI BANK
7	8	-0.3426	0.00	0.00	0.00	DEG K	SIMSCI BANK
7	9	0.0233	0.00	0.00	0.00	DEG K	SIMSCI BANK
8	9	-0.0300	0.00	0.00	0.00	DEG K	SIMSCI BANK
9	10	-7.800E-03	0.00	0.00	0.00	DEG K	SIMSCI BANK

이성분계에 실험데이터로부터 BIP를 선정하는 과정

Example) ISOTHERMAL P,T,X,Y OF CARBON DIOXIDE + ETHANE AT 220.00 K (2) - 20 PTS

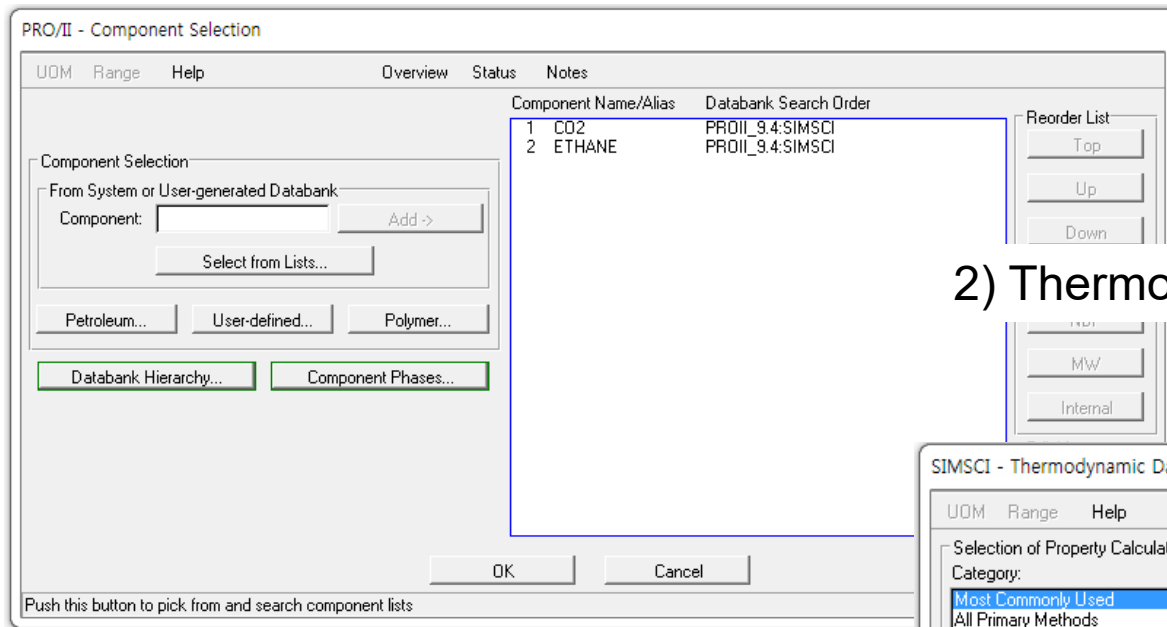
T(K)	P(kPa)	X	Y
220	491.00	0	0
220	522.00	0.015	0.0706
220	548.00	0.0317	0.1239
220	579.00	0.0532	0.1846
220	613.00	0.0812	0.2418
220	660.00	0.1332	0.3178
220	686.00	0.1608	0.3592
220	720.00	0.2186	0.412
220	742.00	0.2564	0.4454
220	765.00	0.319	0.485
220	780.00	0.3693	0.5114
220	796.00	0.4631	0.5518
220	803.00	0.5641	0.5866
220	802.00	0.6552	0.6186
220	788.00	0.7782	0.6692
220	763.00	0.8572	0.7195
220	736.00	0.9035	0.7668
220	700.00	0.9428	0.8247
220	654.00	0.9772	0.9006
220	598.00	1	1



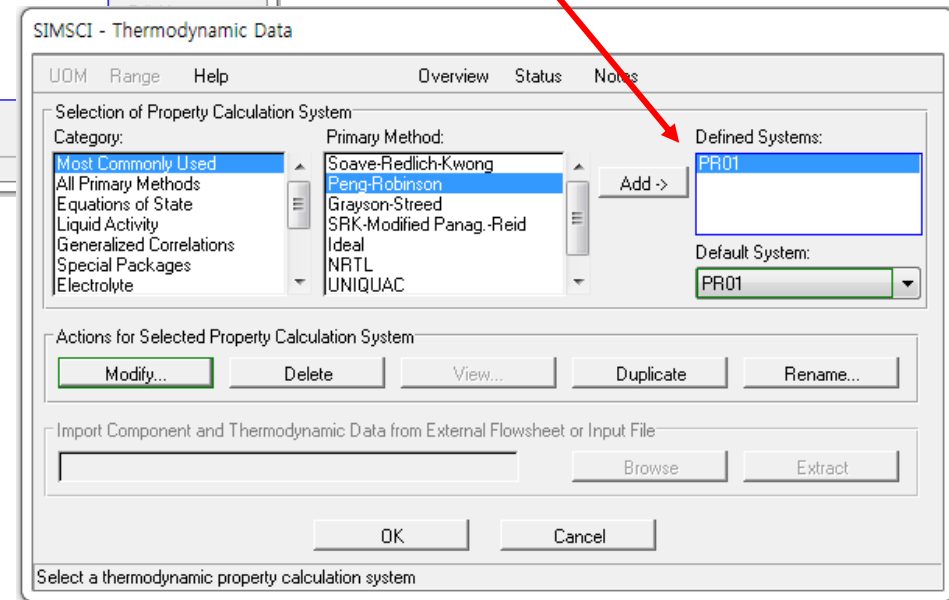
Ref. :BROWN T.S.,KIDNAY A.J.,SLOAN E.D., FLUID PHASE EQUILIB., 40,169(1988)

이성분계에 실험데이터로부터 BIP를 선정하는 과정

1) Component Selection: CO₂와 C₂H₆

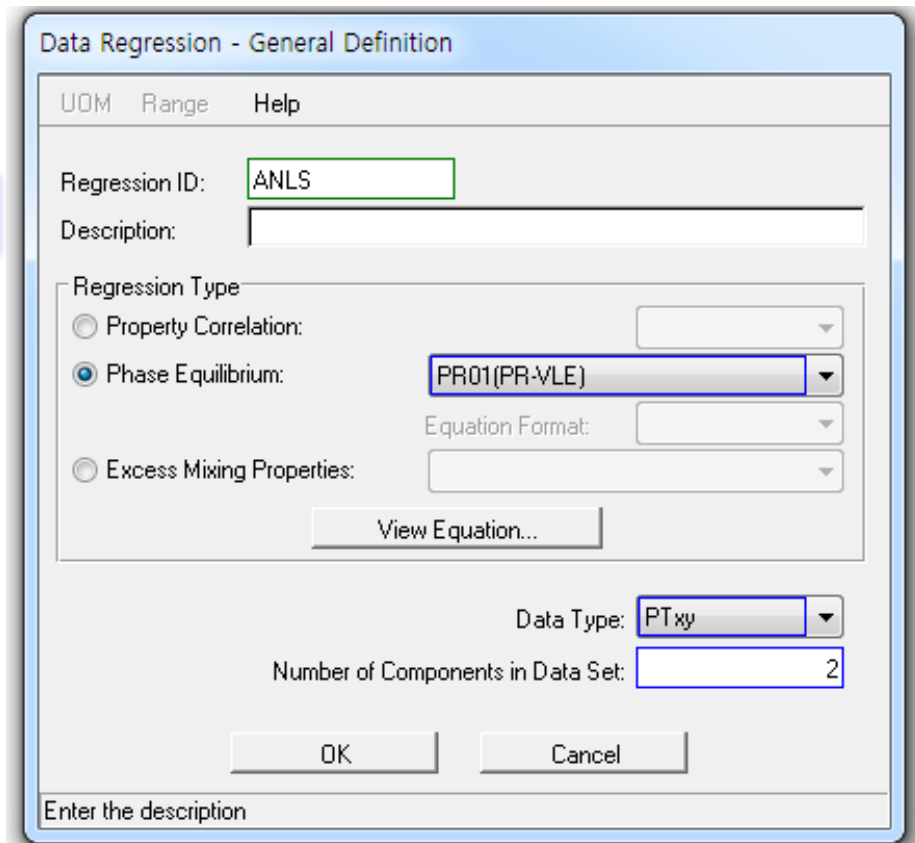
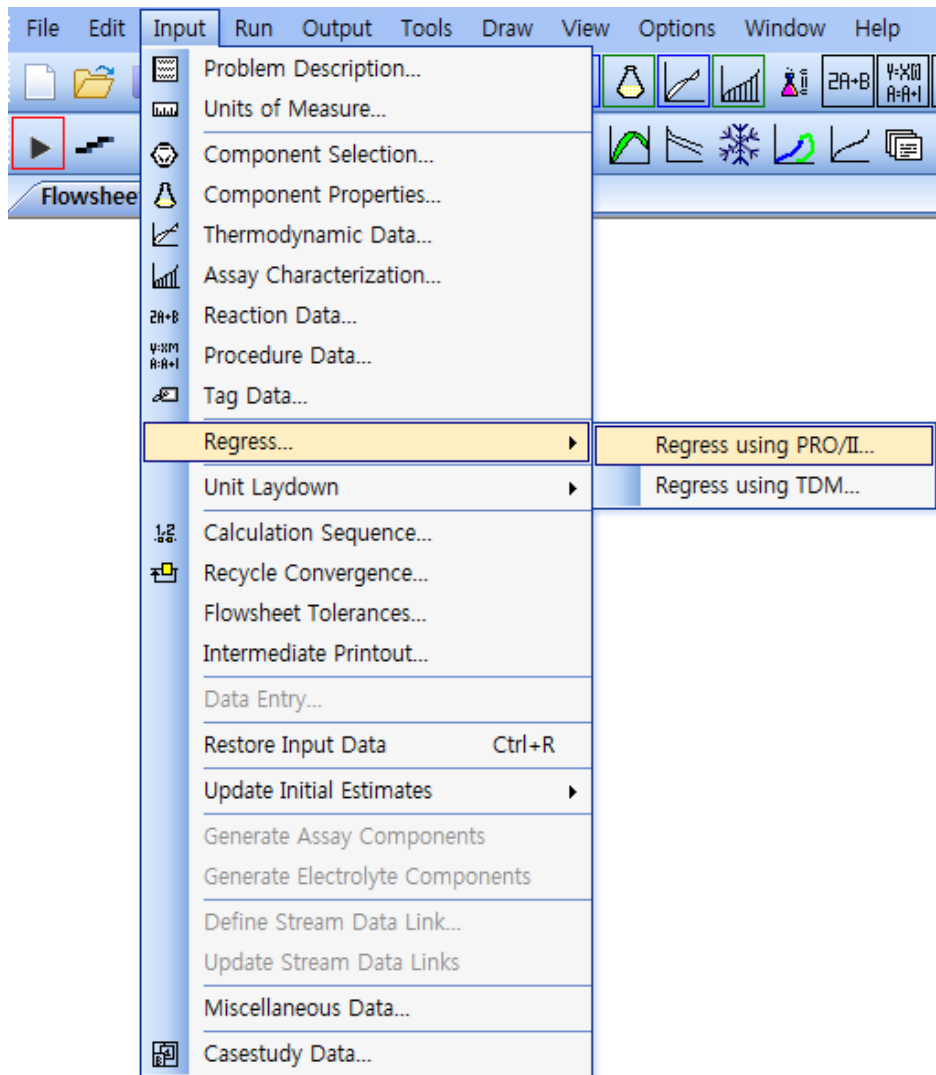


2) Thermodynamic Model Selection: PR



이성분계에 실험데이터로부터 BIP를 선정하는 과정

3) Input → Regress → Regress using PRO/II...



이성분계에 실험데이터로부터 BIP를 선정하는 과정

4) Experimental Data를 입력

Data Regression - Equilibrium Data

UOM Range Help

Name: RAWDATA Description:

Data Source:

Cut	Pressure kPa	Temperature K	x (mol. fract.) for CO2	x (mol. fract.) for ETHANE
Reset 1	491	220	0	
2	522	220	0.015	
3	548	220	0.0317	
4	579	220	0.0532	
5	613	220	0.0812	
6	660	220	0.1332	
7	686	220	0.1608	

OK Cancel

Push this button to accept data entry.

5) 초기값 입력

PRO/II - Data Regression

UOM Range Help Overview

Regression ID: ANLS
Description:

Regression Specification
Regression Type: Equilibrium Data Regression

Data Format: PTxy
Number of Components: 2

Experimental Data...
Objective Function...
Print Options...
View Equation...

Correlation Parameters

i - j Components	Binary Parameters		Initial Estimates	Calculated Values
CO2 - ETHANE	k_{ija}	Not Fixed	0.1322	
	k_{ijb}	Fixed	0	
	k_{ijc}	Fixed	0	

Verify Initial Estimates... Generate Initial Estimates...

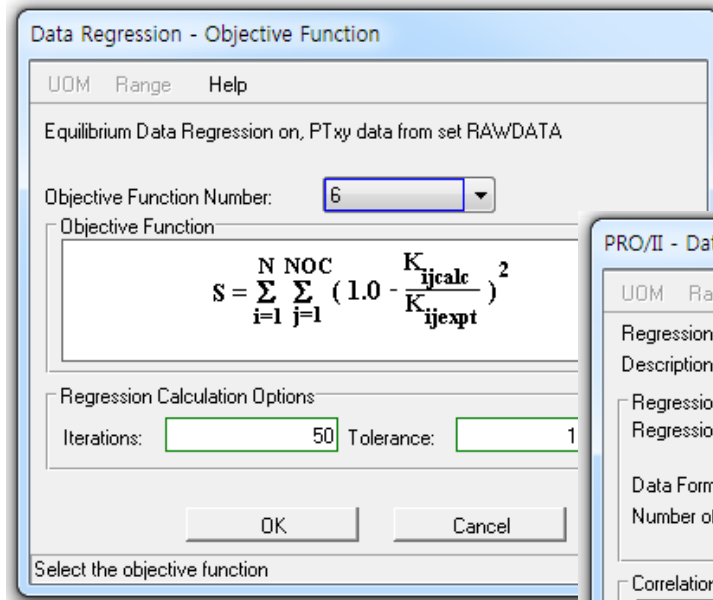
Run Regression View Results... Store Results

Clear the regression data OK Cancel

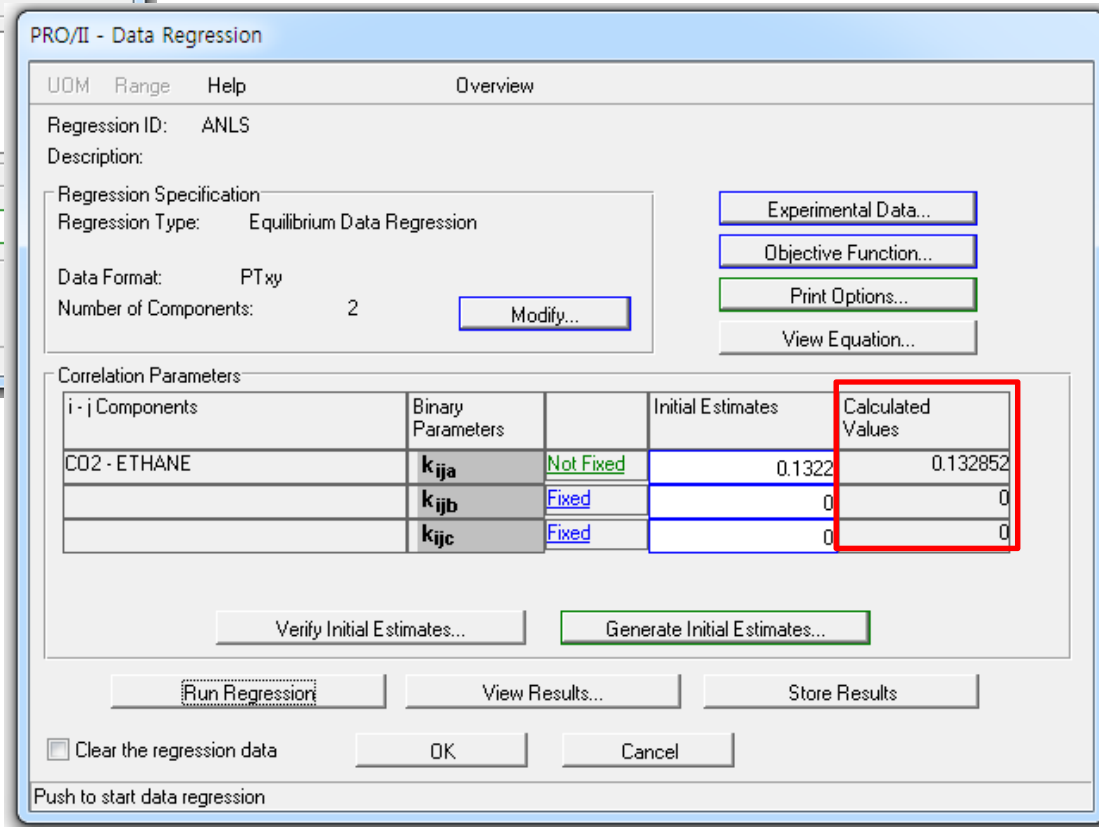
Push this button to accept data entry.

이성분계에 실험데이터로부터 BIP를 선정하는 과정

6) 목적함수의 선택



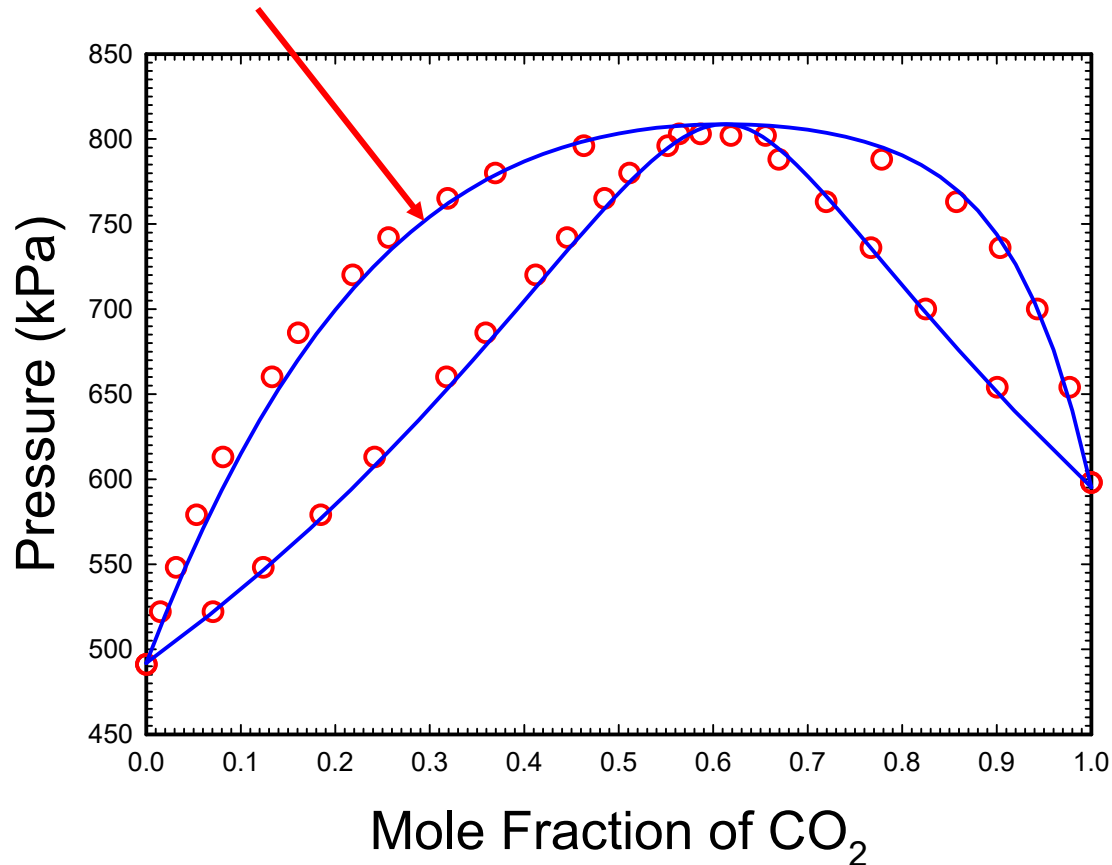
7) View Results에서 Regressed Parameters를 얻는다.



이성분계에 실험데이터로부터 BIP를 선정하는 과정

ISOTHERMAL P,T,X,Y OF CARBON DIOXIDE + ETHANE AT 220.00 K (2) - 20 PTS

Regressed Parameters를 통해 주산한 결과



물성연구에 사용된 천연가스 구성 성분들

• Number of Systems for Each Binary Pairs

	N_2	CO_2	CH_4	C_2H_6	C_3H_8	iC_4H_{10}	nC_4H_{10}
N_2		Set No. 1	Set No. 2	Set No. 3	Set No. 4	Set No. 5	Set No. 6
CO_2			Set No. 7	Set No. 8	Set No. 9	Set No. 10	Set No. 11
CH_4				Set No. 12	Set No. 13	Set No. 14	Set No. 15
C_2H_6					Set No. 16	Set No. 17	Set No. 18
C_3H_8						Set No. 19	Set No. 20
iC_4H_{10}							Set No. 21
nC_4H_{10}							

천연가스 구성성분들의 순수성분 물성

• Pure Component Fixed Properties

Simulator	Properties	Unit	N ₂	CO ₂	CH ₄	C ₂ H ₆	C ₃ H ₈	iC ₄ H ₁₀	nC ₄ H ₁₀
Critical Temperature	HYSYS	K	126.19	304.10	190.69	305.42	369.89	408.09	425.19
	PRO/II		126.20	304.21	190.56	305.32	369.83	408.14	425.12
	Aspen Plus		126.20	304.21	190.56	305.32	369.83	407.80	425.12
Critical Pressure	HYSYS	kPa	3,394.37	7,370.00	4,640.68	4,883.85	4,256.66	3,647.62	3,796.62
	PRO/II		3,400.00	7,383.00	4,599.00	4,872.00	4,248.00	3,648.00	3,796.00
	Aspen Plus		3,400.00	7,383.00	4,599.00	4,872.00	4,248.00	3,640.00	3,796.00
Acentric Factor	HYSYS	-	0.03998	0.23894	0.01155	0.09860	0.15240	0.18479	0.20100
	PRO/II		0.03772	0.22362	0.01155	0.09949	0.15229	0.18077	0.20016
	Aspen Plus		0.03772	0.22362	0.01154	0.09949	0.15229	0.18352	0.20016

각각의 이성분계 쌍에 대한 BIP's

➤ BIP's Built-in P2, A+, HYSYS & DECHEMA

	N2	CO2	CH4	C2H6	C3H8	iC4H10	nC4H10
N2		-0.0170	0.0350	0.0500	0.0800	0.0900	0.0900
		-0.0170	0.0311	0.0515	0.0852	0.1033	0.0800
		-0.0200	0.0360	0.0500	0.0800	0.0950	0.0900
		-0.0200	0.0300	0.0440	0.0780	0.1000	0.0870
CO2			0.0919	0.1322	0.1241	0.1200	0.1333
			0.0919	0.1322	0.1241	0.1200	0.1333
			0.1000	0.1298	0.1350	0.1298	0.1298
			0.0900	0.1300	0.1200	0.1300	0.1350
CH4				-0.0026	0.0140	0.0256	0.0133
				-0.0026	0.0140	0.0256	0.0133
				-0.00224	0.00683	0.01311	0.01230
				-0.0030	0.0160	0.0260	0.0190
C2H6					0.0011	-0.0067	0.0096
					0.0011	-0.0067	0.0096
					0.00126	0.00457	0.00410
					0.0010	-0.0070	0.0100
C3H8						-0.0078	0.0033
						-0.0078	0.0033
						0.00104	0.00082
						-0.0070	0.0030
iC4H10							-0.0004
							-0.0004
							0.00001
							0.0000

P2
A+
HYSYS
DECHEMA

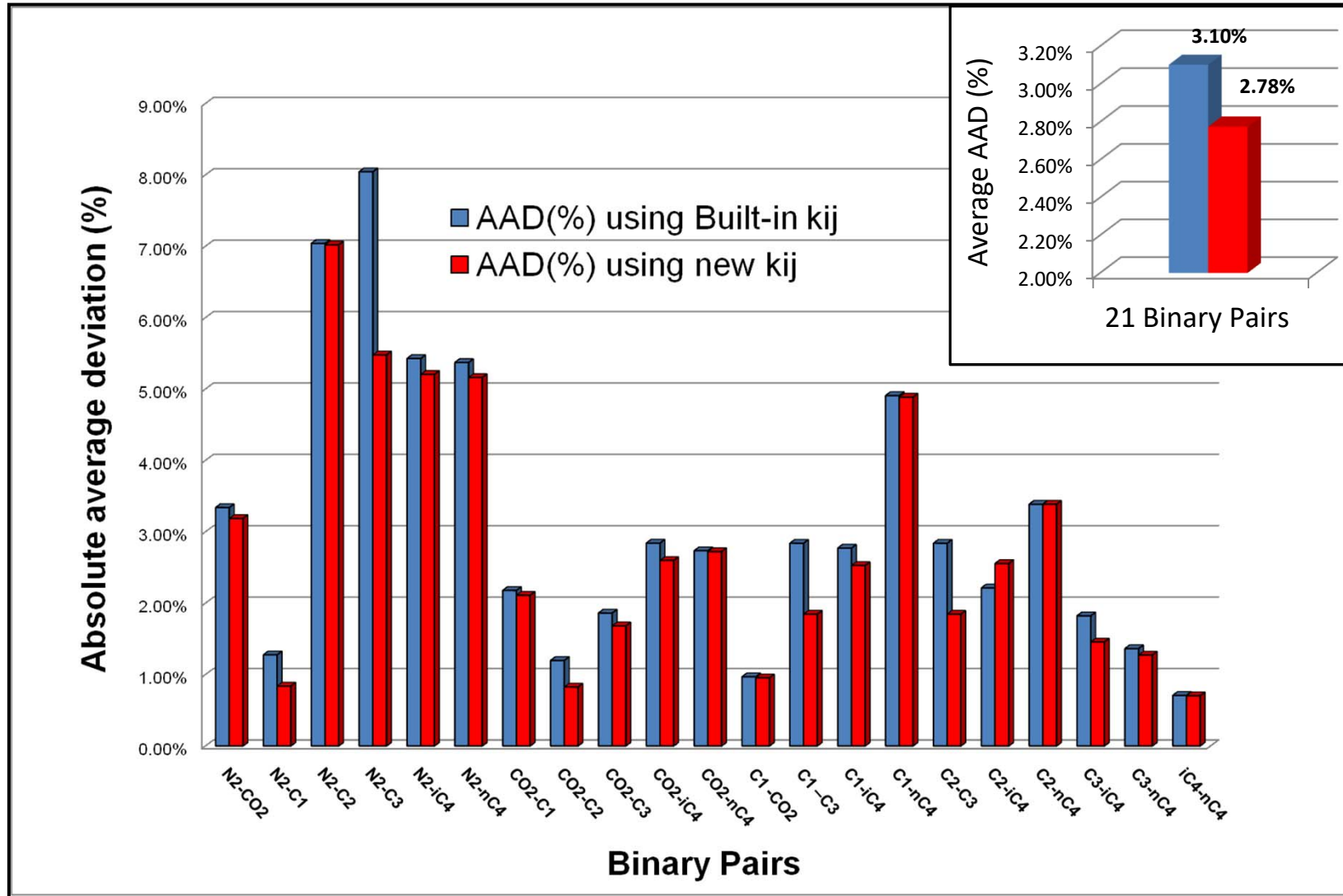
Searching for Experimental VLE Data:

- Isothermal vapor-liquid equilibrium data in DECHEMA DB for each binary pairs containing N_2 , CO_2 , CH_4 , C_2H_6 , C_3H_8 , iC_4H_{10} , nC_4H_{10}

	N_2	CO_2	C_1	C_2	C_3	IC_4	NC_4
N_2		54	145	102	45	16	31
CO_2			96	69	41	15	67
C_1				106	86	12	106
C_2					70	20	33
C_3						45	27
IC_4							36
NC_4							

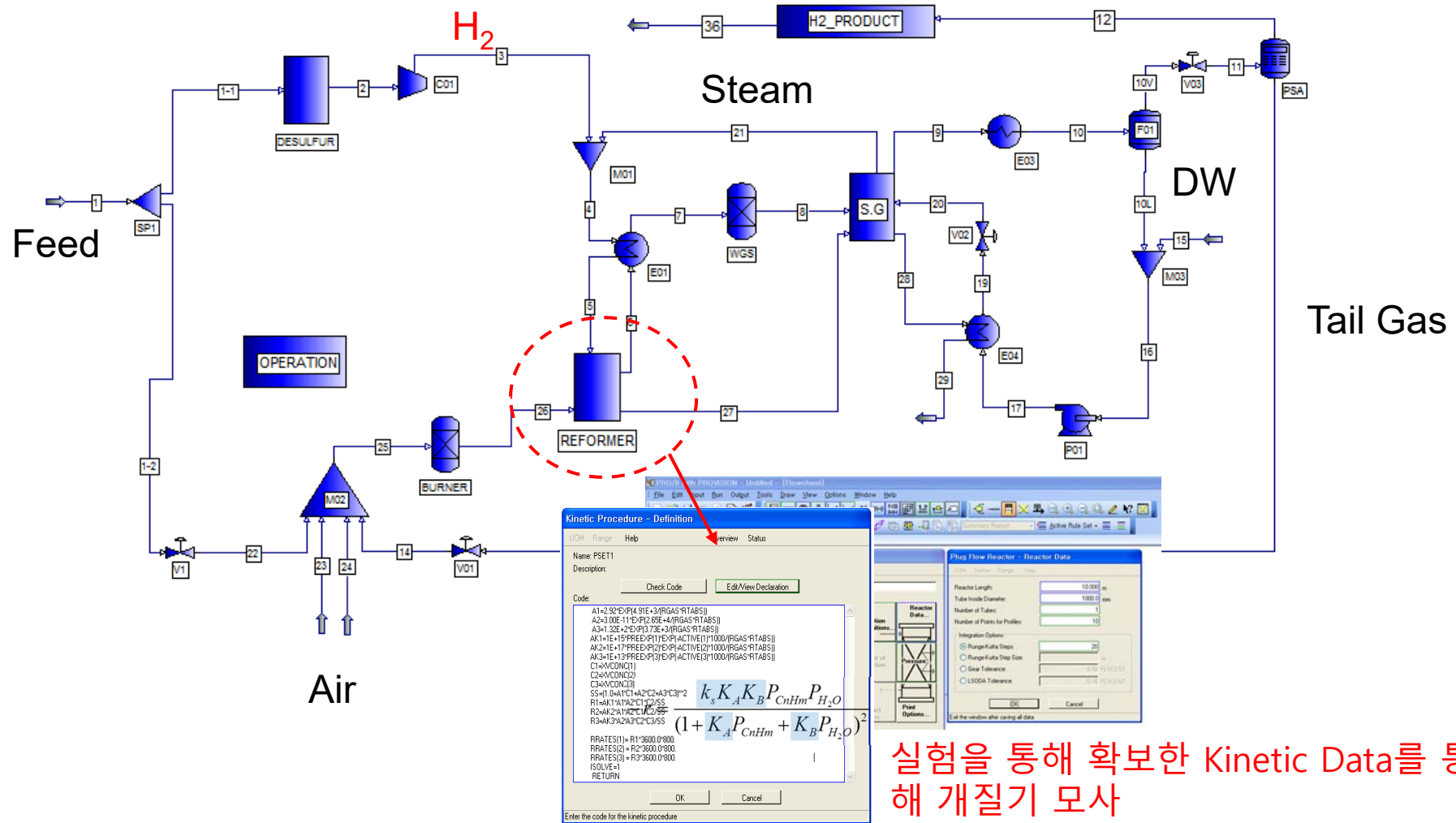
Total: 1,222 Binary Experimental Isothermal Binary Data !!!

상평형 물성 개선 결과



Case 2(Typical 2)전산모사 결과

상용성 화학공정 모사기(PRO/II 10.0)를 사용하여, 500 kg/day 수소생산공정에 대한 **공정 모사**



실험을 통해 확보한 Kinetic Data를 통해 개질기 모사

Stream Summary:

STREAM ID	R_T	101	102	103
NAME		Feed		
PHASE	WET VAPOR	DRY VAPOR	DRY VAPOR	DRY VAPOR
THERMO ID	SRK01	SRK01	SRK01	SRK01
FLUID RATES, KG/HR				
1 C1	2.6557	56.0418	52.5497	52.5497
2 H2O	142.0109	0.0000	0.0000	0.0000
3 C2	0.2090	5.0670	4.7513	4.7513
4 C3	1.1756E-07	2.5321	2.3743	2.3743
5 NC4	5.9209E-11	1.5270	1.4318	1.4318
6 CO	102.8608	0.0000	0.0000	0.0000
7 H2	21.5378	0.0000	0.0000	0.0000
8 CO2	0.0000	0.0000	0.0000	0.0000
9 N2	0.1972	0.2103	0.1972	0.1972
10 O2	0.0000	0.0000	0.0000	0.0000
TOTAL RATE, KG/HR	269.4714	65.3781	61.3042	61.3042
TEMPERATURE, C	885.0000	20.0000	20.0000	19.8937
PRESSURE, BAR(GA)	3.7000	1.0001	1.0001	0.8000
ENTHALPY, M*KCAL/HR	0.2418	3.9368E-03	3.6915E-03	3.6915E-03
MOLECULAR WEIGHT	12.0200	17.4203	17.4203	17.4203
WEIGHT FRAC VAPOR	1.0000	1.0000	1.0000	1.0000
WEIGHT FRAC TOTAL LIQUID	0.0000	0.0000	0.0000	0.0000

Stream Summary:

STREAM ID		112	113	114	115
NAME		SynGas		H2	
PHASE		WET VAPOR	WET VAPOR	WET VAPOR	WET VAPOR
THERMO ID		SRK01	SRK01	SRK01	SRK01
FLUID RATES, KG/HR					
1	C1	2.6557	2.6557	4.1445E-04	4.1445E-04
2	H2O	2.1310	2.1310	1.8616E-04	1.8616E-04
3	C2	0.2090	0.2090	3.1073E-04	3.1073E-04
4	C3	1.1756E-07	1.1756E-07	1.1756E-07	1.1756E-07
5	NC4	5.9209E-11	5.9209E-11	0.0000	0.0000
6	CO	40.3214	40.3214	1.0131E-03	1.0131E-03
7	H2	26.0387	26.0387	20.8310	20.8310
8	CO2	98.2616	98.2616	4.5478E-04	4.5478E-04
9	N2	0.1972	0.1972	0.0000	0.0000
10	O2	0.0000	0.0000	0.0000	0.0000
TOTAL RATE, KG/HR		169.8146	169.8146	20.8334 (500 kg/day)	20.8333
TEMPERATURE, C		24.1979	24.1515	27.1611	692.3550
PRESSURE, BAR(GA)		3.3000	2.8000	1.8000	63.9868
ENTHALPY, M*KCAL/HR		0.0103	0.0103	1.0070E-03	0.0496
MOLECULAR WEIGHT		10.0560	10.0560	2.0161	2.0161
WEIGHT FRAC VAPOR		1.0000	1.0000	1.0000	1.0000
WEIGHT FRAC TOTAL LIQUID		0.0000	0.0000	0.0000	0.0000

20.8334 x 24
500.0016 kg/day

Stream Summary:

STREAM ID		112	113	114	115
NAME		SynGas		H2	
PHASE		WET VAPOR	WET VAPOR	WET VAPOR	WET VAPOR
THERMO ID		SRK01	SRK01	SRK01	SRK01
FLUID NORMAL GAS PERCENTS					
1	C1	0.9803	0.9803	2.5000E-04	2.5000E-04
2	H2O	0.7005	0.7005	1.0000E-04	1.0000E-04
3	C2	0.0412	0.0412	1.0000E-04	1.0000E-04
4	C3	1.5787E-08	1.5787E-08	2.5799E-08	2.5799E-08
5	NC4	6.0323E-12	6.0323E-12	0.0000	0.0000
6	CO	8.5245	8.5245	3.5000E-04	3.5000E-04
7	H2	76.4903	76.4903	99.9991	99.9991
8	CO2	13.2217	13.2217	1.0000E-04	1.0000E-04
9	N2	0.0417	0.0417	0.0000	0.0000
10	O2	0.0000	0.0000	0.0000	0.0000
TOTAL RATE, M3/HR		378.5015	378.5015	231.6155	231.6155
TEMPERATURE, C		24.1979	24.1515	27.1611	692.3550
PRESSURE, BAR(GA)		3.3000	2.8000	1.8000	63.9868
ENTHALPY, M*KCAL/HR		0.0103	0.0103	1.0070E-03	0.0496
MOLECULAR WEIGHT		10.0560	10.0560	2.0161	2.0161
MOLE FRAC VAPOR		1.0000	1.0000	1.0000	1.0000
MOLE FRAC LIQUID		0.0000	0.0000	0.0000	0.0000