천연가스 구성 성분들에 대한 물성 및 열역학적 모델식 소개

2020년 2월 11일(화)

공주대학교 화학공학부

조 정 호

목 차

1 천연가스 구성 성분들의 고정 물성

2 Aspen HYSYS 내의 Peng-Robinson 모델식의 BIP’s Regression

3 Fortran을 이용한 다양한 목적함수 Regression

4 GERG-2008 모델식과 다른 모델식 사이의 비교

1 천연가스 구성 성분들의 고정 물성

천연가스(Natural Gas)란?

- 주성분은 메탄(CH_4)이고, 에탄(C_2H_6) 함량이 많고 적음에 따라서 rich gas와 lean gas로 구분한다.
- 천연가스 처리공정의 3개의 키워드:
  - Purification(전처리 공정)
    - 천연가스 중의 불순물: 이산화탄소, 황화수소, 수분, 수은 등
    - 불순물 제거 공정: AGRU, Dehydration Process 등
  - Volume Reduction(액화공정: Liquefaction Process)
    - 천연가스를 액화시키는 이유
    - 부피가 600분의 1로 줄어들기 때문에 저장 및 수송이 용이하다.
    - 동일한 저장 부피에 600배 많은 천연가스를 저장할 수 있다.
    - 이송시에 가스배관보다 액체 배관의 직경이 더 작다.
    - 기체 이송시에 압축기를 사용하는 것 보다 액체 이송 시에 펌프를 사용하면 동력을 줄일 수 있다.
  - Separation(NGL 회수공정)
    - 에탄 이상의 성분을 회수하는 공정

천연가스 구성 성분들:

- 천연가스 구성 성분들:
  - CO_2: 불순물로 AGRU 공정에 의해서 제거되어야 할 성분
  - H_2O: 불순물로 Dehydration 공정에 의해서 제거되어야 할 성분
  - N_2: 천연가스 구성성분 중의 하나이지만 열량가는 없음
  - CH_4: 대부분을 차지하는 성분임
  - C_2H_6: 에탄 함량의 많고 적음에 따라서 Rich와 Lean으로 나뉘어짐
  - C_3H_8: 소량 존재
  - Iso-C_4H_{10}: 미량 존재
  - N-C_4H_{10}: 미량 존재

3가지 기본적인 물성들:

- 3 Most Fundamental Fixed Properties:
  - Molecular Weight
  - Standard Liquid Density
  - Normal Boiling Point

Component	MW (kg/k-mol)	Density (kg/m^3)	NBP (^{o}C)
N_2	28.0135	807.96	-195.81
CO_2	44.0098	816.43	-78.48
CH_4	16.0428	299.70	-161.49
C_2H_6	30.0696	355.04	-88.60
C_3H_8	44.0965	505.79	-42.04
Iso-C_4H_{10}	58.1234	563.84	-11.72
N-C_4H_{10}	58.1234	584.33	-0.50

2

Aspen HYSYS 내의 Peng-Robinson 모델식의 BIP's Regression

천연가스 구성 성분들의 물성:

➤ Critical Properties:

Simulator	Properties	Unit	N_2	CO_2	CH_4	C_2H_6	C_3H_8	iC_4H_{10}	nC_4H_{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 and 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

물성 연구에 사용된 천연가스 구성 성분들:

- Number of Systems for Each Binary Pairs:

21 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}							

Peng-Robinson Equation of State:

The PR equation is represented by:

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)-b(v-b)}$$

Peng-Robinson Equation of State

where:

$$a = a_c \alpha$$

$$a_c = 0.45724 \frac{R^2 T_c^2}{P_c} \qquad b = 0.07780 \frac{RT_c}{P_c}$$

The alpha function to estimate pure component vapor pressure is shown:

$$\alpha = \left[1 + \kappa\left(1 - \sqrt{T_r}\right)\right]^2 \qquad \kappa = 0.37464 + 1.5422\omega - 0.26992\omega^2$$

Peng-Robinson Equation of State:

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

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

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

Regressed binary interaction parameter

- Mixing Rule 1: $k_{ij} = a_{ij}$
- Mixing Rule 2: $k_{ij} = 1 - a_{ij} + \frac{b_{ij}}{T}$
- Mixing Rule 3: $k_{ij} = 1 - a_{ij} + b_{ij}T$

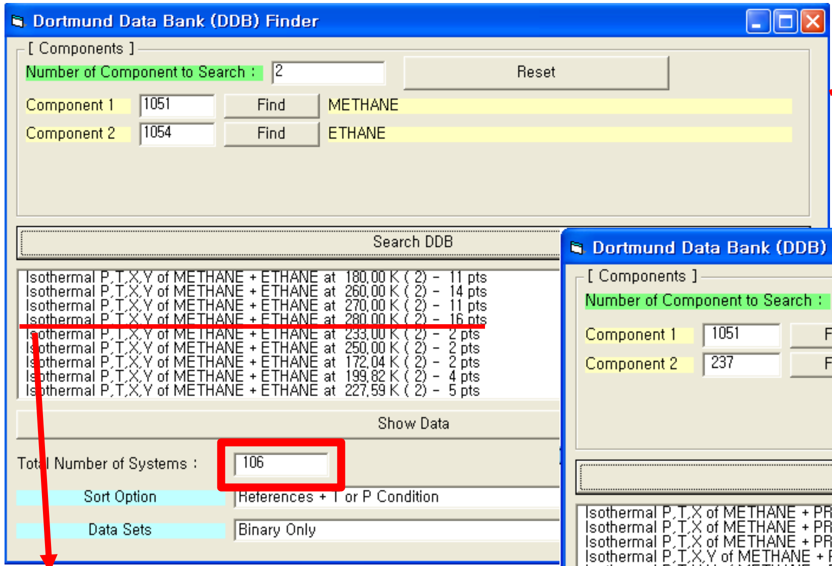
Searching for Experimental VLE Data:

- 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}

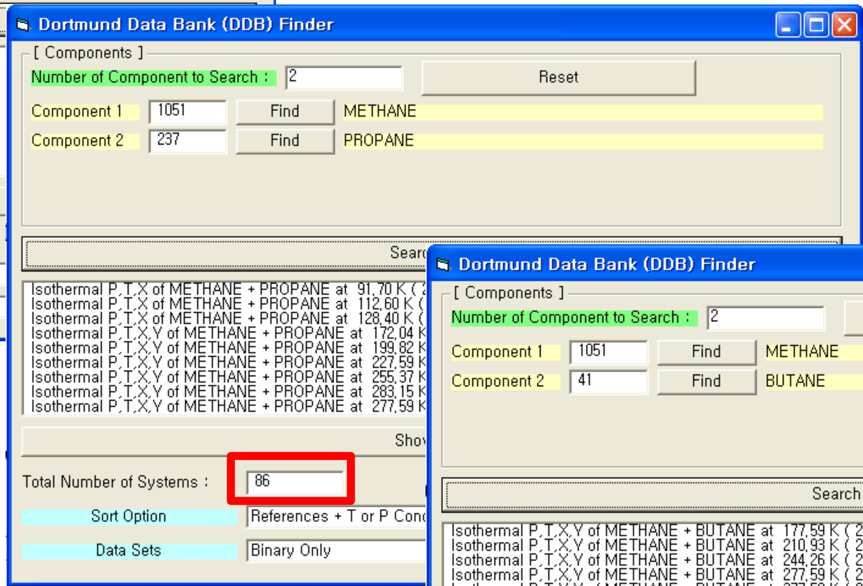
	N_2	CO_2	C_1	C_2	C_3	IC_4	NC_4
N_2		54	145	102	45	16	31
CO_2			96	69	41	15	67
C_1				106	86	12	106
C_2					70	20	33
C_3						45	27
IC_4							36
NC_4							

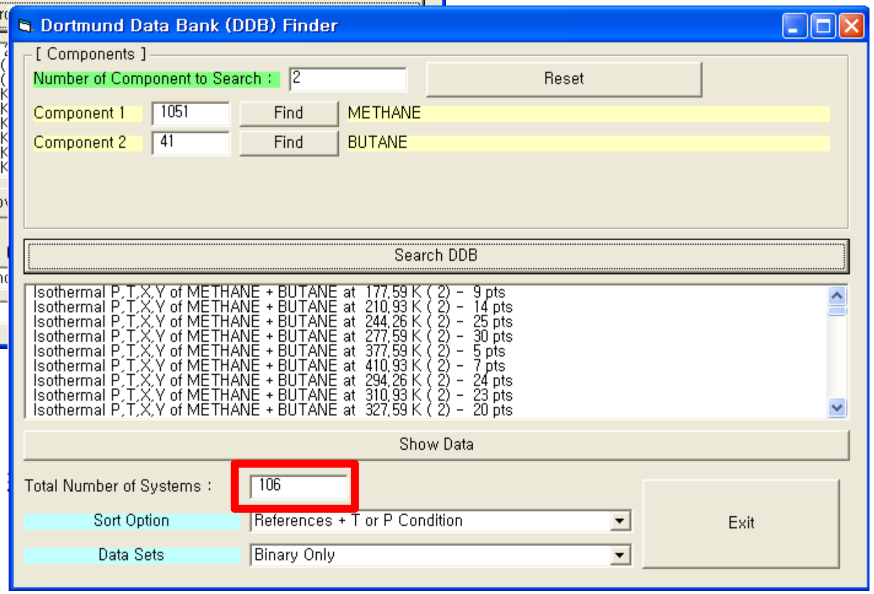
Total: 1,222 Binary Experimental Isothermal Binary Data !!!

Binary Experimental VLE Data:



Over 100 binary pairs are available in DECHEMA DB for C1-C3 pair.





T(K)	P(kPa)	X	Y
280	2796.6	0.0000	0.0000
280	2887.8	0.0081	0.0279
280	3075.2	0.0231	0.0744
280	3203.9	0.0335	0.1036
280	3655.8	0.0693	0.1864
280	4037.8	0.0996	0.2404
280	4415.7	0.1292	0.2818
280	4711.6	0.1528	0.3091
280	5040.9	0.1798	0.3336
280	5329.7	0.2044	0.3512
280	5645.8	0.2333	0.3654
280	5984.3	0.2668	0.3719
280	6086.6	0.2774	0.3711
280	6191.0	0.2913	0.3675
280	6265.9	0.3046	0.3609
280	6292.3	0.3109	0.3557

ISOTHERMAL P,T,X,Y OF METHANE + ETHANE AT 280.00 K (2) – 16 PTS

Reference: GUPTA M.K.,GARDNER G.C.,HEGARTY M.J.,KIDNAY A.J., J.CHEM.ENG.DATA, 25,313(1980)

VLE Data Regression: Objective Functions

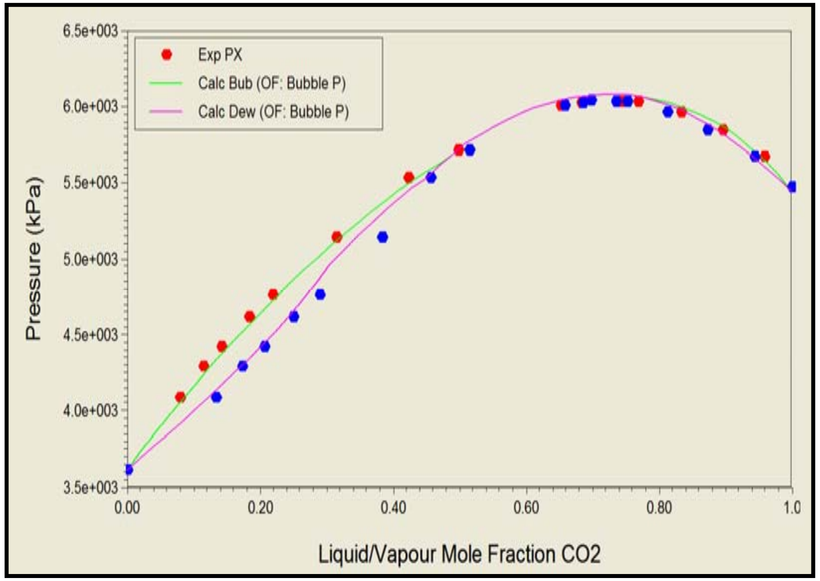
Bubble Pressure

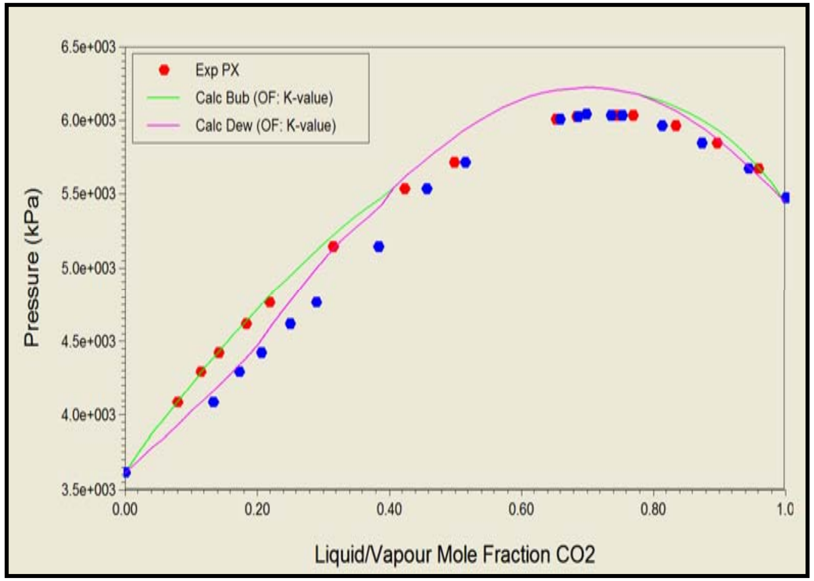
$$Obj. = \sum_{j=1}^{N} \left(\frac{P_j^{\exp} - P_j^{cal}}{P_j^{\exp}} \right)^2$$

K-Value

$$Obj. = \sum_{j=1}^{N} \left(\frac{K_j^{\exp} - K_j^{cal}}{K_j^{\exp}} \right)^2$$

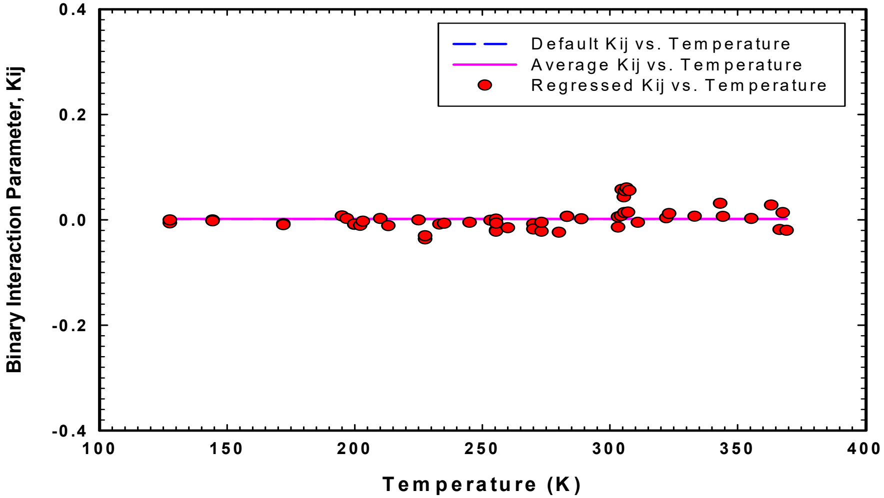
이 경우에는 **Bubble Pressure** 추산을 다소 희생시켜야 함



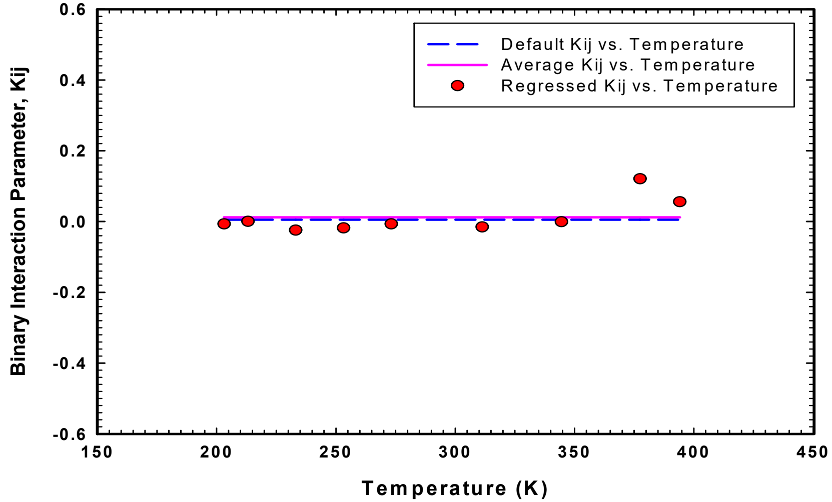


Result: Regressed BIP's vs. Temperature

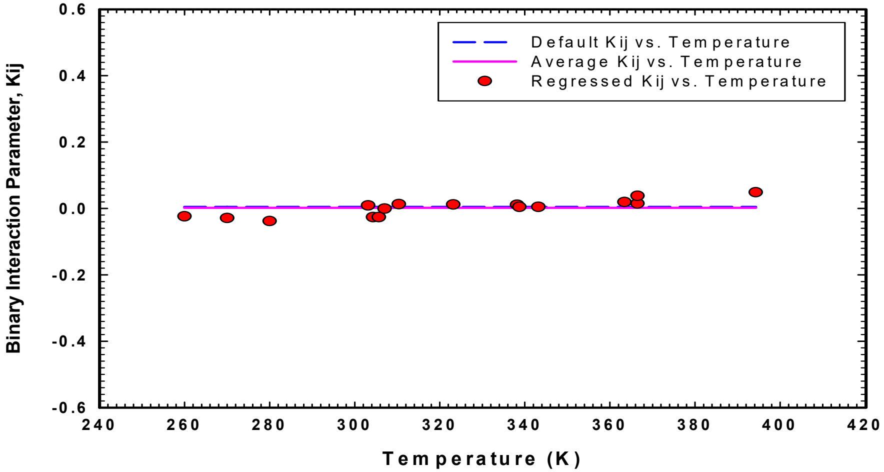
- C_2H_6-C_3H_8 System



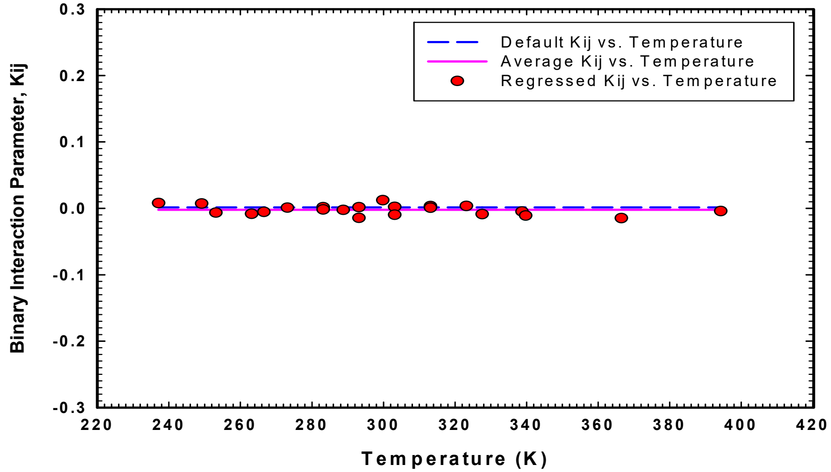
- C_2H_6-iC_4H_{10} System



- C_2H_6-nC_4H_{10} System

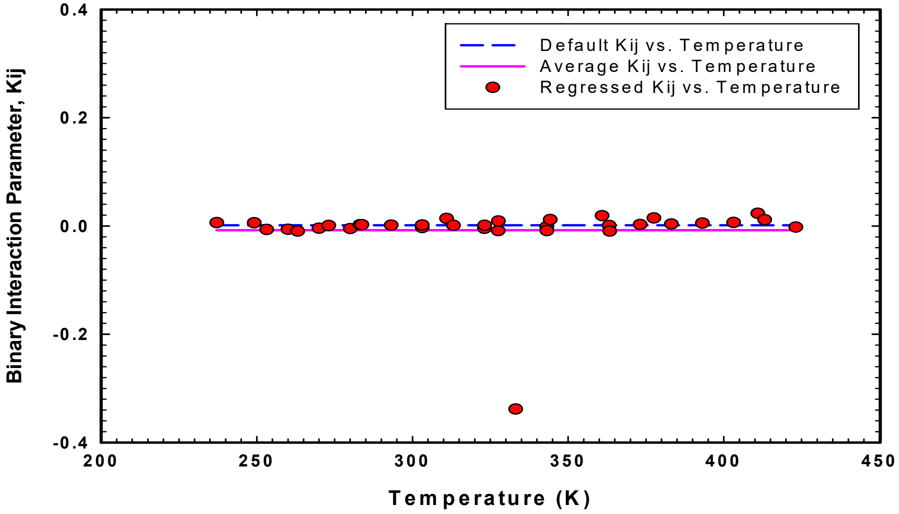


- C_3H_8-nC_4H_{10} System

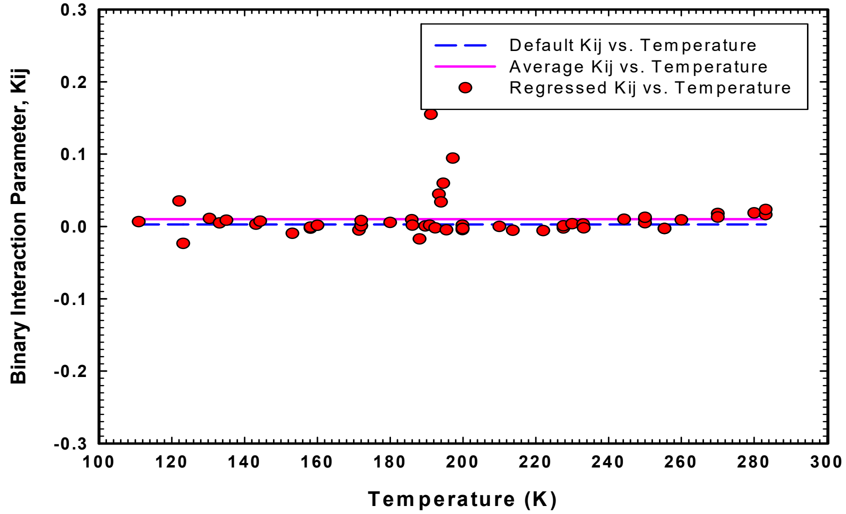


Result: Regressed BIP's vs. Temperature

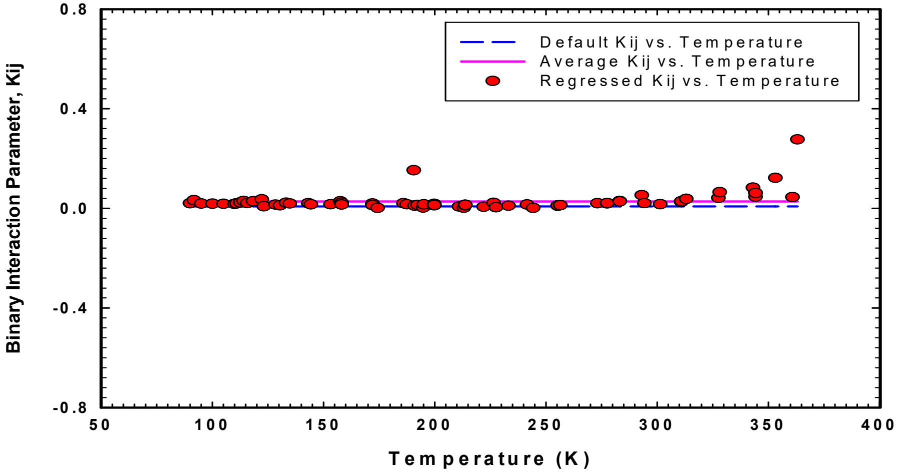
➢ C_3H_8-nCH_4 System



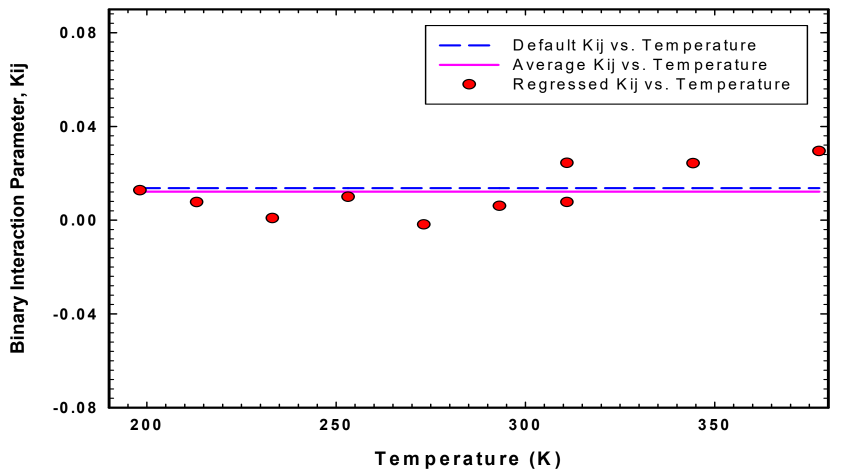
➢ CH_4-C_2H_6 System



➢ CH_4-C_3H_8 System

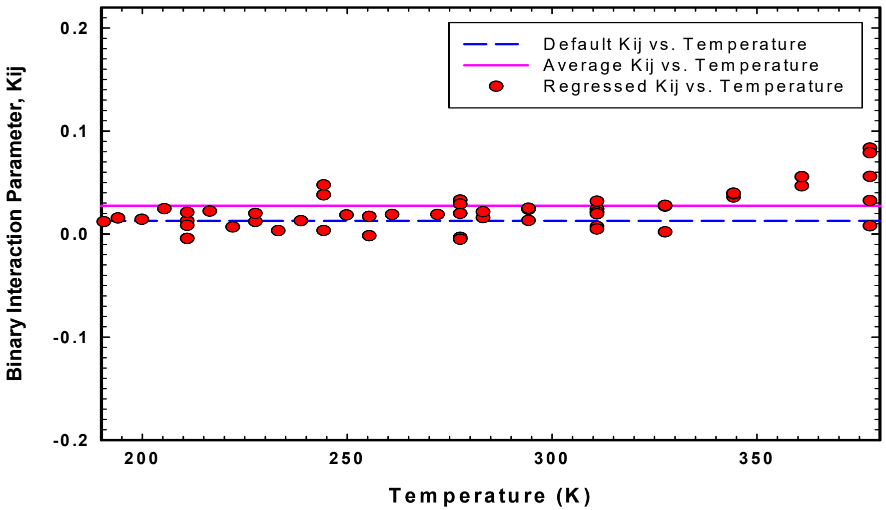


➢ CH_4-iC_4H_{10} System

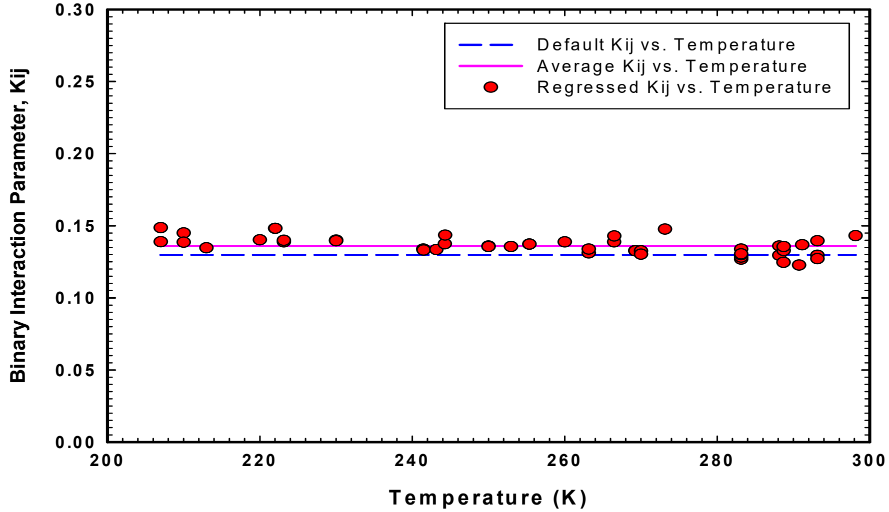


Result: Regressed BIP's vs. Temperature

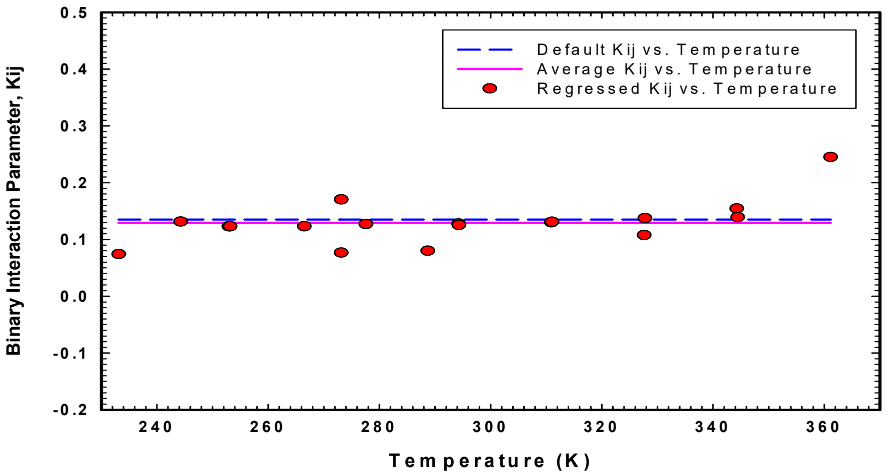
➢ CH_4-nC_4H_{10} System



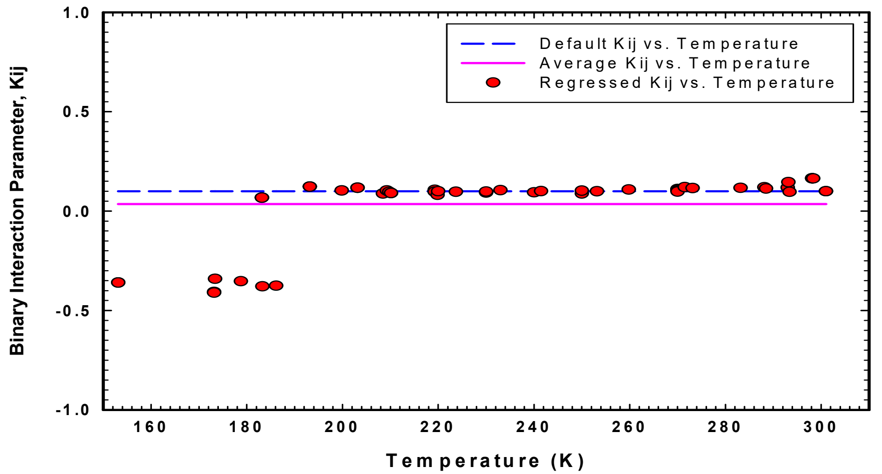
➢ CO_2-C_2H_6 System



➢ CO_2-C_3H_8 System

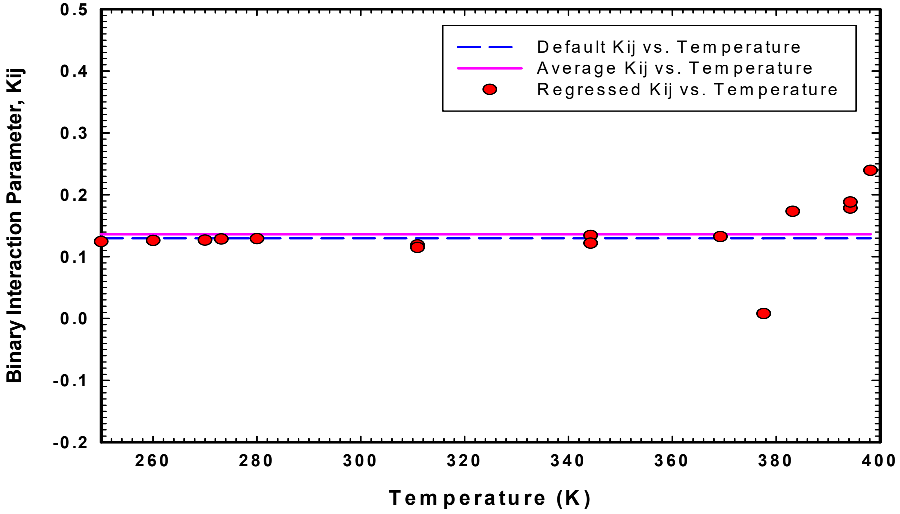


➢ CO_2-CH_4 System

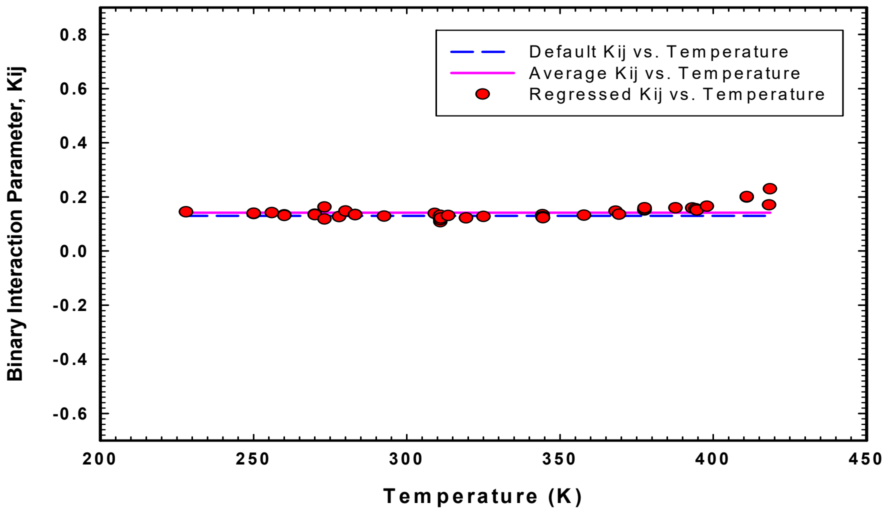


Result: Regressed BIP's vs. Temperature

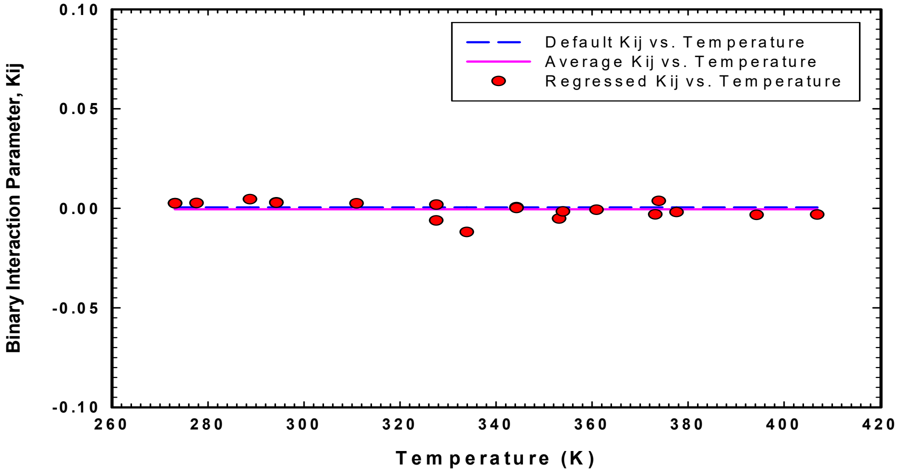
➢CO_2-iC_4H_{10} System



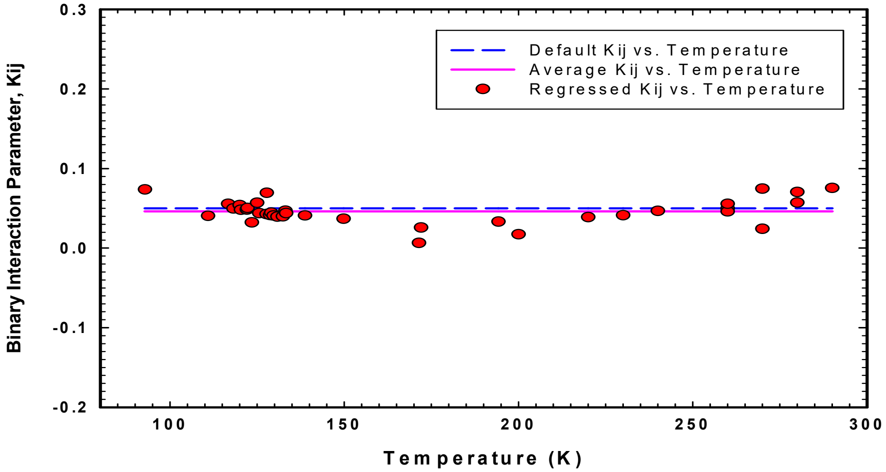
➢CO_2-nC_4H_{10} System



➢iC_4H_{10}-nC_4H_{10} System

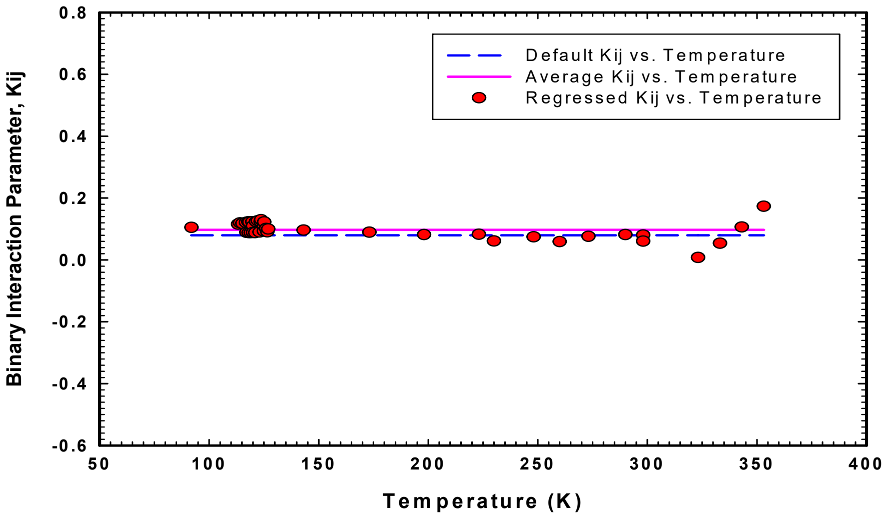


➢ N_2-C_2H_6 System

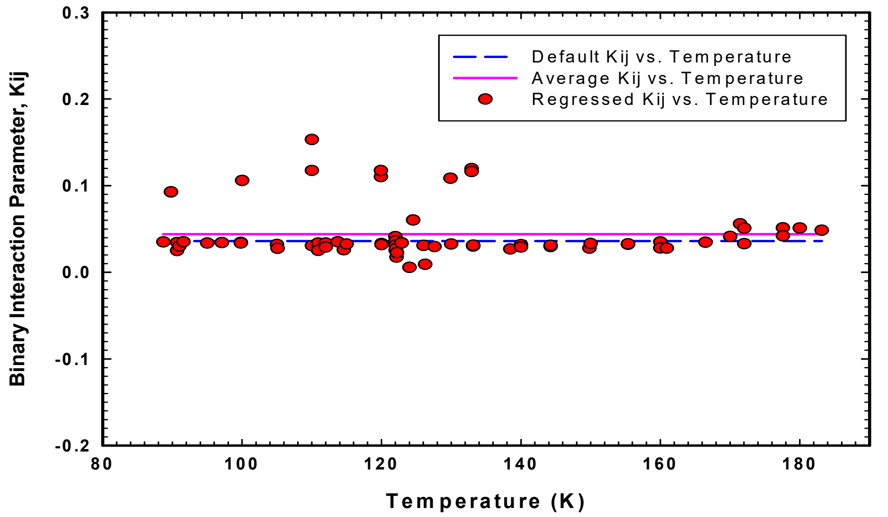


Result: Regressed BIP's vs. Temperature

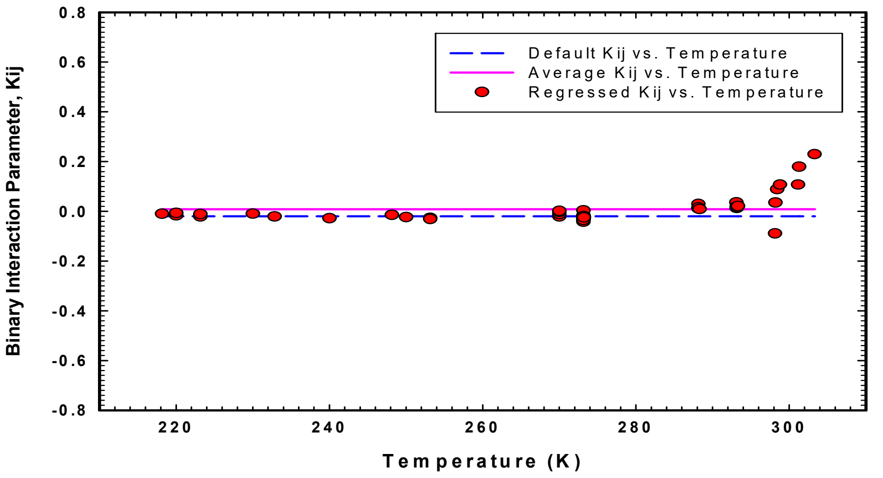
➢ N_2-C_3H_8 System



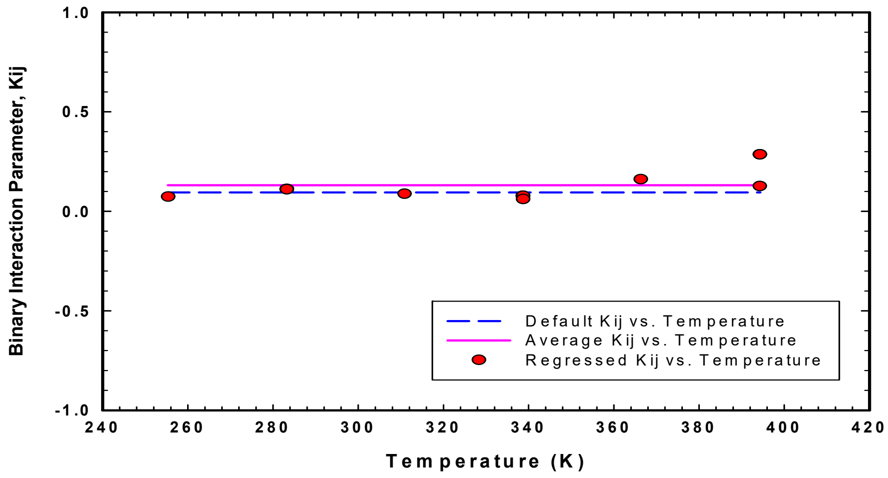
➢ N_2-CH_4 System



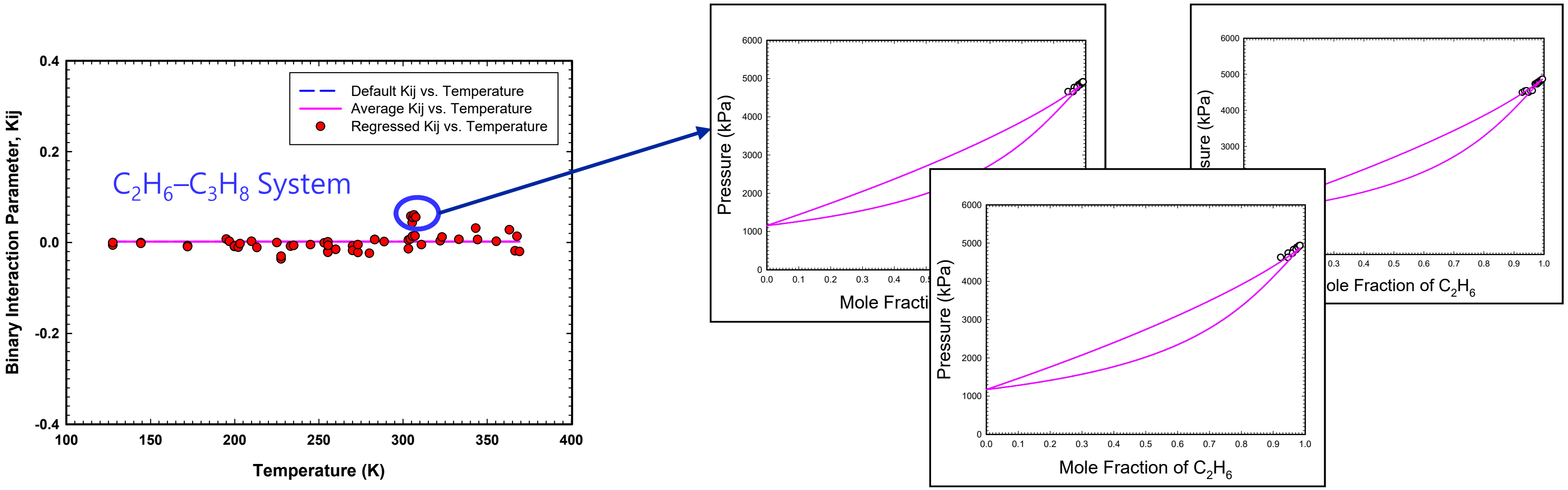
➢ N_2-CO_2 System

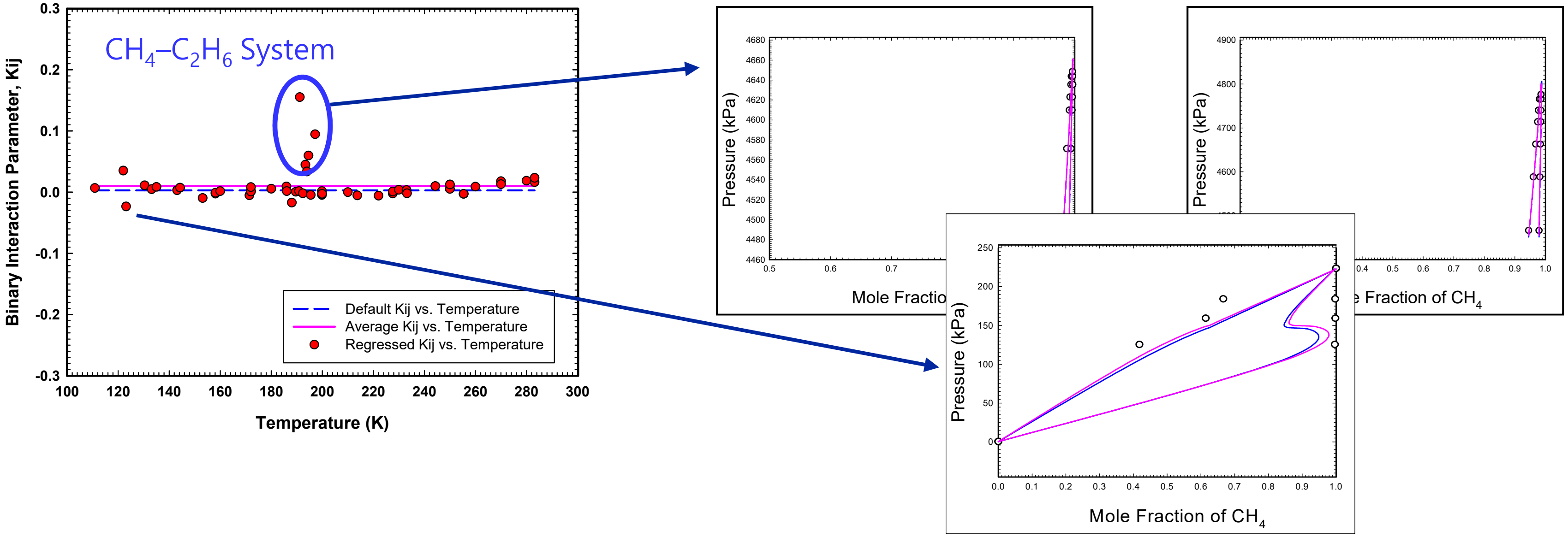


➢ N_2-iC_4H_{10} System



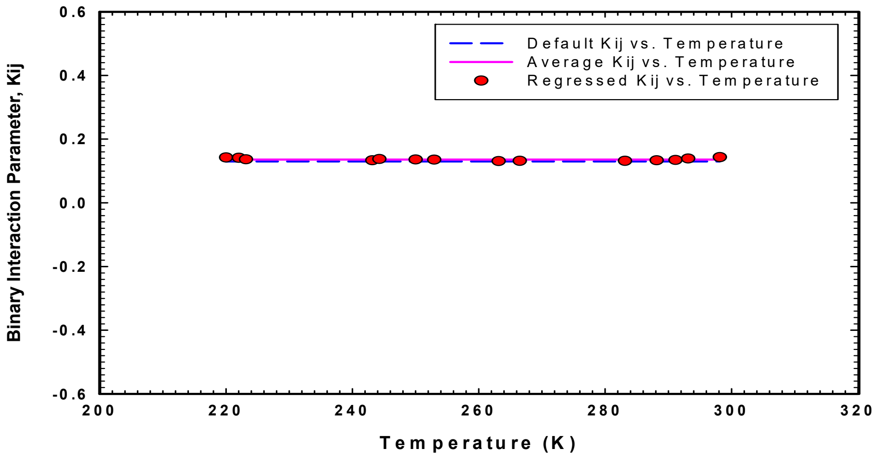
부정확한 실험 데이터 제외:



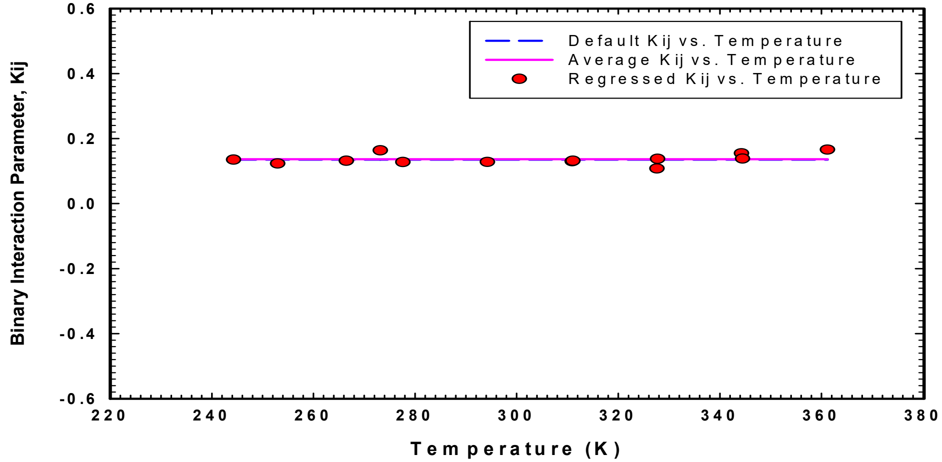


Result: Regressed BIP's vs. Temperature (개선 후)

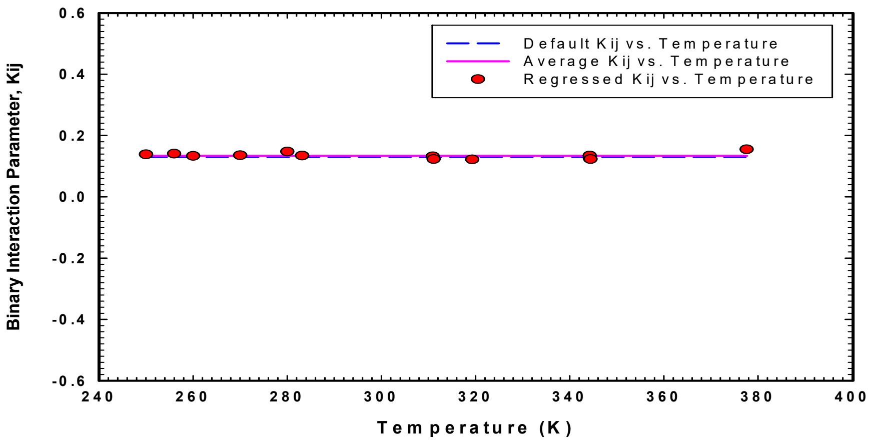
➢CO_2-C_2H_6 System



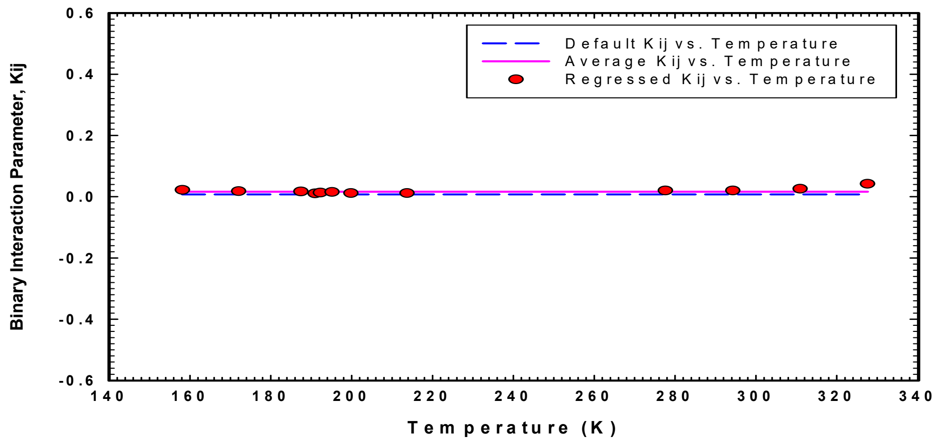
➢CO_2-C_3H_8 System



➢CO_2-nC_4H_{10} System

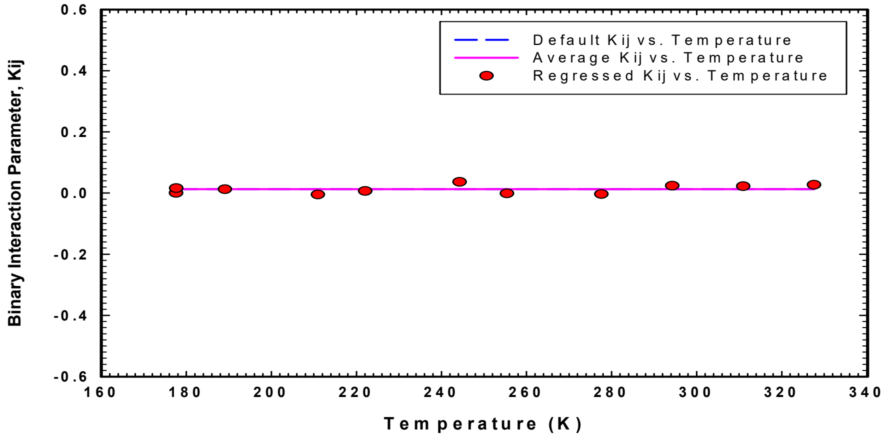


➢ CH_4-C_3H_8 System

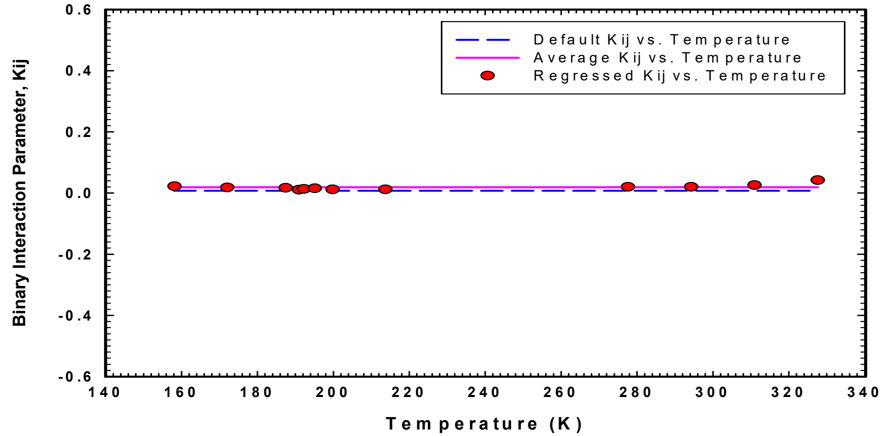


Result: Regressed BIP's vs. Temperature (개선 후)

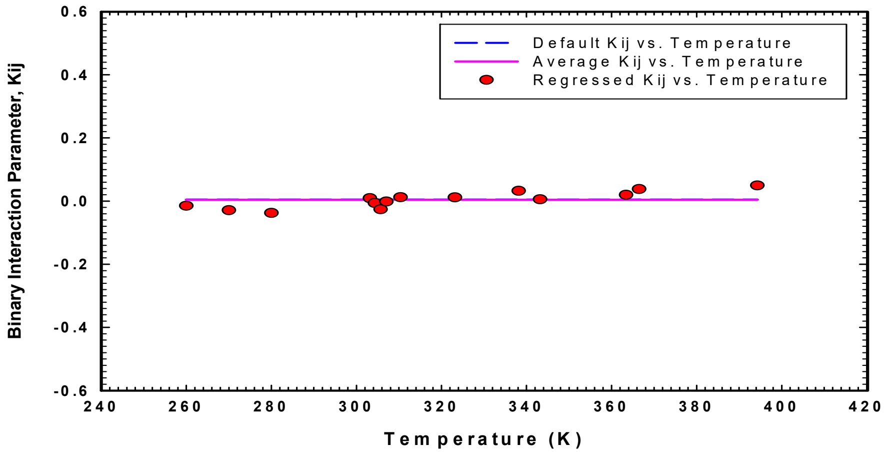
- CH_4-nC_4H_{10} System



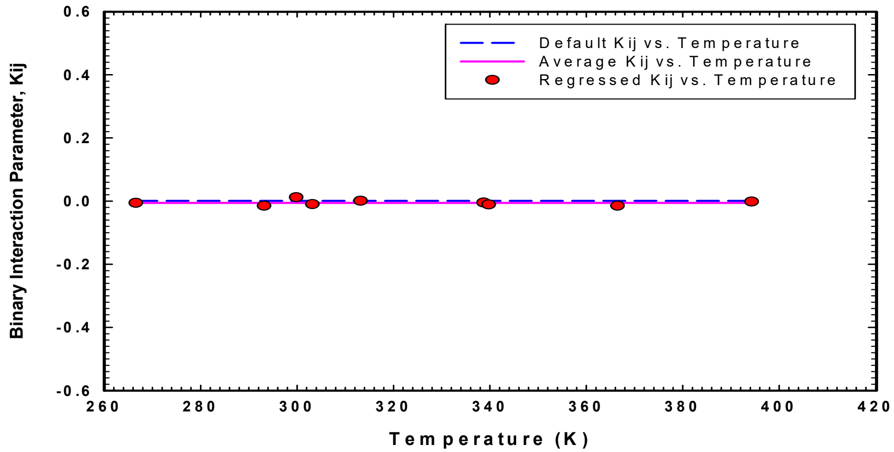
- C_2H_6-C_3H_8 System



- C_2H_6-nC_4H_{10} System



- C_3H_8-iCH_{10} System



Result: kij Built-in HYSYS & Bew Regressed kij:

	N_2	CO_2	C_1	C_2	C_3	IC_4	NC_4
N_2		-0.0200	0.0360	0.0500	0.0800	0.0950	0.0900
		0.0080	0.0440	0.0461	0.0973	0.1311	0.0962
CO_2			0.1000	0.1298	0.1350	0.1298	0.1298
			0.0358	0.1360	0.1290	0.1363	0.1418
C_1				-0.00224	0.00683	0.01311	0.0123
				0.0100	0.0282	0.0120	0.0273
C_2					0.00126	0.00457	0.0041
					0.1290	0.1360	0.0022
C_3						0.00104	0.00082
						-0.00227	-0.0077
IC_4							0.00001
							0.0004725
NC_4							

kij Built-in HYSYS (first row of each pair)

New kij (second row of each pair)

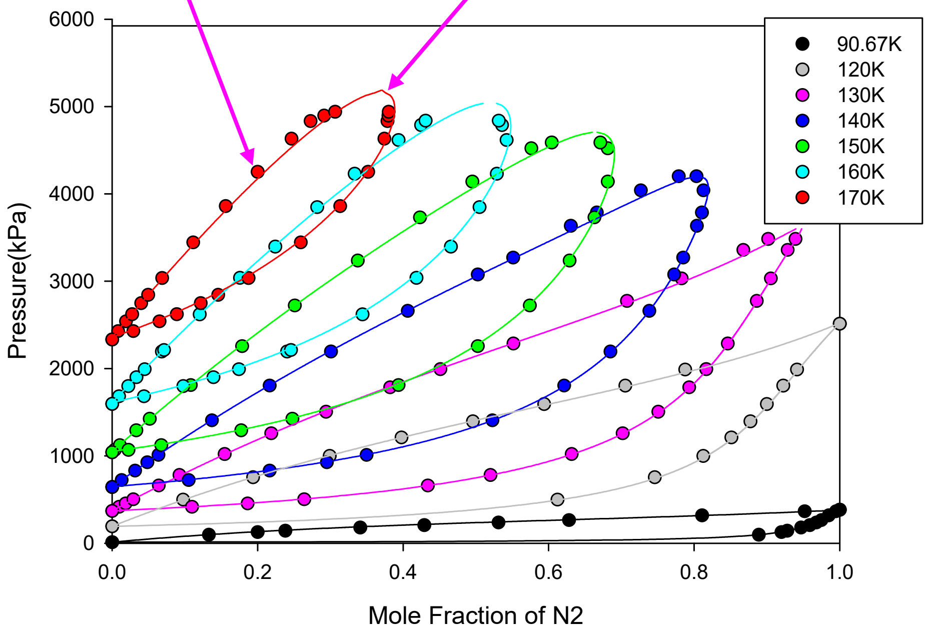
Result: Comparison of AAD(%) vetween kij built-in HYSYS and New kij

AAD(absolute average deviation) (%)

$$AAD(\%) = \sum_{j=1}^{N} \left| \frac{P_j^{\exp} - P_j^{cal}}{P_j^{\exp}} \right| \times 100$$

Dot ted: 실험 Data

Line: New kij 값을 사용하여 추산한 결과

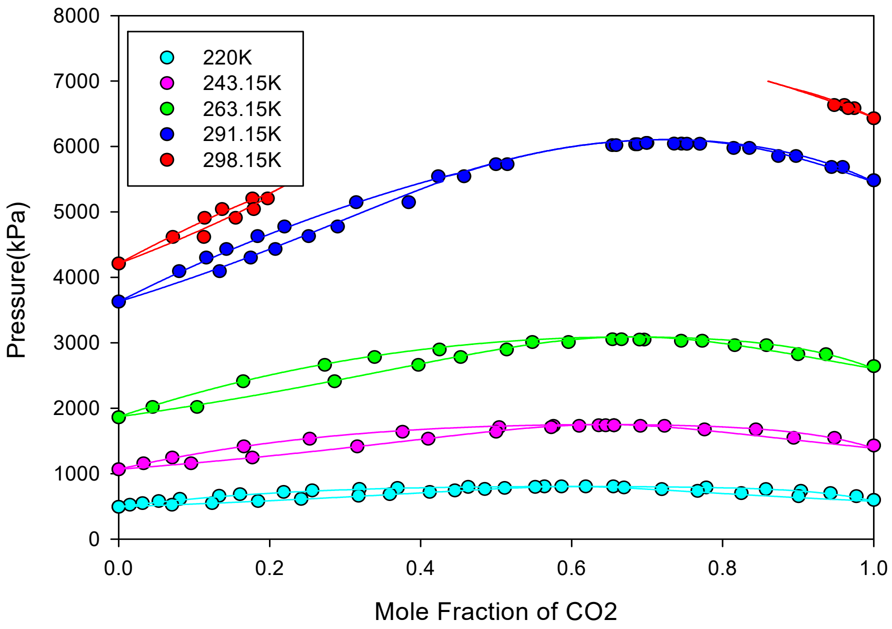


Temperature (K)	N_2-CH_4 AAD(%)	
	k_{ij} built-in HYSYS	new k_{ij}
90.67	4.449%	2.787%
100.00	0.989%	0.686%
115.00	0.836%	0.417%
120.00	1.142%	0.570%
127.59	0.885%	0.652%
130.00	1.006%	0.710%
133.15	1.597%	0.990%
138.46	1.525%	0.824%
140.00	1.124%	0.705%
144.26	1.457%	0.682%
149.82	1.306%	0.882%
150.00	0.920%	0.731%
153.37	0.681%	0.288%
160.00	0.865%	0.779%
160.93	1.275%	1.111%
166.48	0.476%	0.562%
170.00	1.172%	0.892%
Average	**1.277%**	**0.839%**

Result: Comparison of AAD(%) vetween kij built-in HYSYS and New kij

AAD(absolute average deviation) (%)

$$AAD(\%) = \sum_{j}^{N} \left| \frac{P_j^{exp} - P_j^{cal}}{P_j^{exp}} \right| \times 100$$

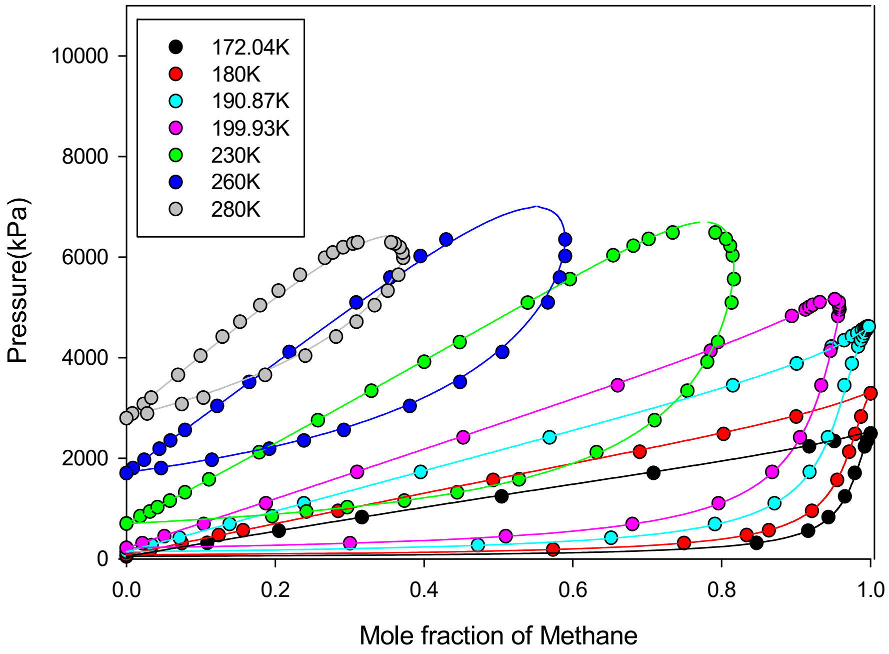


Temperature (K)	CO_2-C_2H_6 AAD(%)	
	k_{ij} built-in HYSYS	new k_{ij}
220.00	2.457%	1.279%
222.04	2.861%	1.294%
223.15	1.643%	0.624%
243.15	0.891%	0.792%
244.26	1.568%	0.776%
250.00	1.193%	0.580%
252.95	1.298%	1.241%
263.15	0.435%	0.853%
266.48	0.824%	0.924%
283.15	0.752%	0.867%
288.15	0.695%	0.656%
291.15	0.664%	0.626%
293.15	0.966%	0.671%
298.15	0.521%	0.375%
Average	**1.198%**	**0.826%**

Result: Comparison of AAD(%) vetween kij built-in HYSYS and New kij

AAD(absolute average deviation) (%)

$$AAD(\%) = \sum_{j}^{N} \left| \frac{P_j^{\exp} - P_j^{cal}}{P_j^{\exp}} \right| \times 100$$

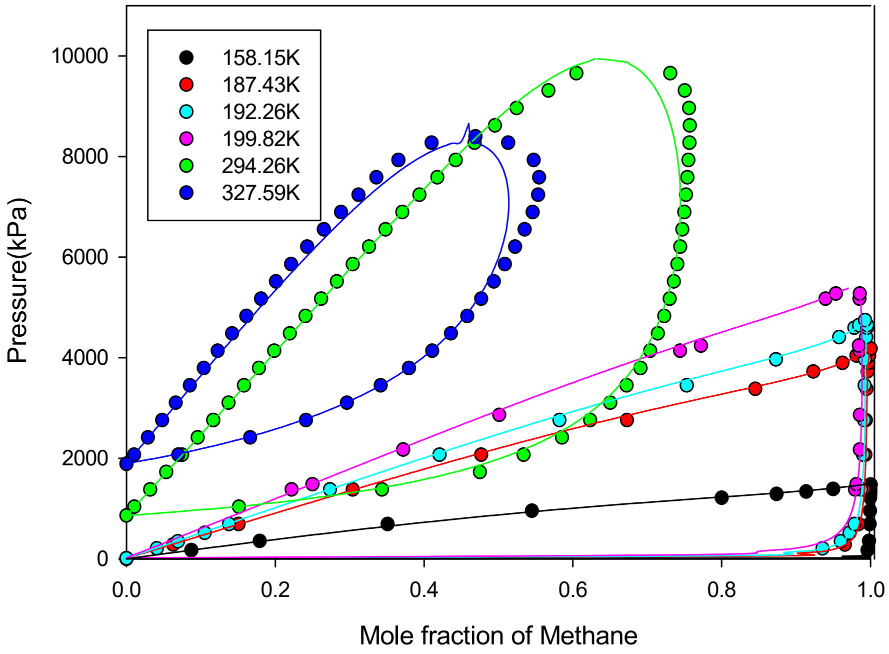


Temperature (K)	CH_4-C_2H_6 AAD(%)	
	k_{ij} built-in HYSYS	new k_{ij}
172.04	1.118%	1.231%
180.00	1.325%	0.880%
190.87	0.636%	0.832%
199.93	1.064%	1.447%
230.00	0.369%	0.345%
260.00	0.844%	0.694%
280.00	1.430%	1.248%
Average	**0.969%**	**0.954%**

Result: Comparison of AAD(%) vetween kij built-in HYSYS and New kij

AAD(absolute average deviation) (%)

$$AAD(\%) = \sum_{j}^{N} \left| \frac{P_j^{\exp} - P_j^{cal}}{P_j^{\exp}} \right| \times 100$$

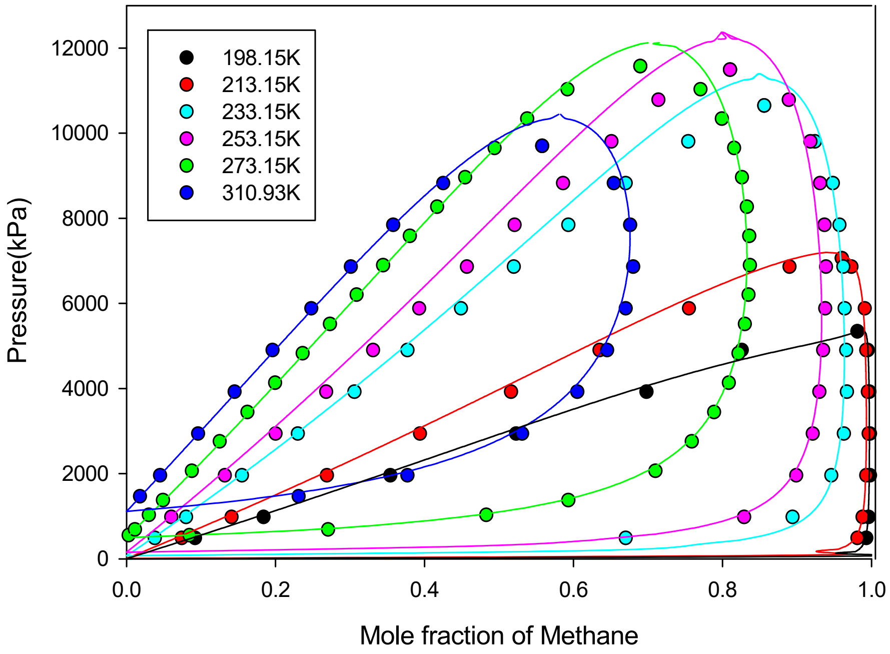


Temperature (K)	CH_4-C_3H_8 AAD(%)	
	k_{ij} built-in HYSYS	new k_{ij}
158.15	6.051%	3.300%
172.04	4.105%	1.984%
187.43	2.588%	1.406%
190.93	1.144%	1.575%
192.26	2.300%	2.202%
195.15	2.706%	1.717%
199.82	2.936%	1.986%
213.71	2.379%	3.281%
277.59	2.620%	1.199%
294.26	2.128%	0.713%
310.93	2.277%	0.951%
Average	**2.840%**	**1.847%**

Result: Comparison of AAD(%) vetween kij built-in HYSYS and New kij

AAD(absolute average deviation) (%)

$$AAD(\%) = \sum_{j}^{N} \left| \frac{P_j^{\exp} - P_j^{cal}}{P_j^{\exp}} \right| \times 100$$



Temperature (K)	CH_4-iC_4H_{10} AAD(%)	
	k_{ij} built-in HYSYS	new k_{ij}
198.15	1.306%	1.287%
213.15	2.256%	1.545%
233.15	4.602%	4.207%
253.15	2.731%	2.556%
273.15	5.030%	3.943%
293.15	2.655%	2.247%
310.93	2.321%	2.805%
310.95	2.495%	2.275%
344.25	1.555%	1.895%
Average	**2.772%**	**2.529%**

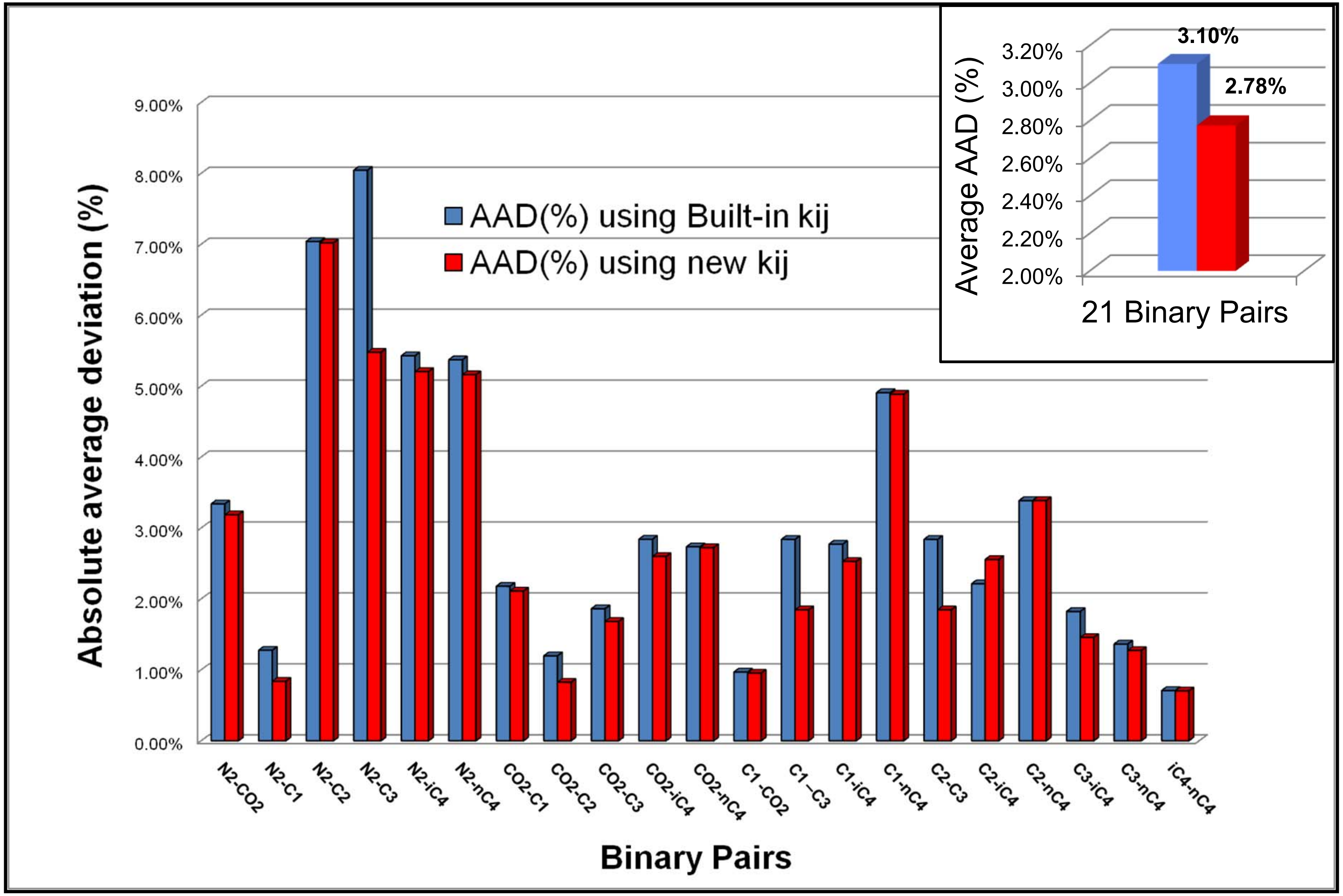
Result: Comparison of AAD(%) vetween kij built-in HYSYS and New kij

	N_2	CO_2	C_1	C_2	C_3	IC_4	NC_4
N_2		3.340%	1.277%	7.040%	8.044%	5.428%	5.372%
		3.187%	0.839%	7.020%	5.478%	5.206%	5.161%
CO_2			2.179%	1.198%	1.862%	2.842%	2.735%
			2.112%	0.826%	1.683%	2.599%	2.723%
C_1				0.969%	2.840%	2.772%	4.909%
				0.954%	1.847%	2.529%	4.887%
C_2					2.840%	2.214%	3.387%
					1.847%	2.556%	3.387%
C_3						1.823%	1.364%
						1.457%	1.274%
IC_4							0.708%
							0.703%
NC_4							

kij Built-in HYSYS

New kij

Result: Comparison of AAD(%) vetween kij built-in HYSYS and New kij



3

Fortran을 이용한 다양한 목적함수 Regression

CO_2-C_2H_6 System에 대해서 우선 적용:

PRO/II

case	Object Function	BIP Mixing Rule	aij	bij	P AAD (%)	y AAD (%)
1_1	Bubble P	kij= aij	*0.1341*		0.9083	2.6029
1_2	Bubble P	kij= aij+bij/T	*0.1123*	*5.2223*	0.8602	2.6051
2_1	Bubble P + y	kij= aij	*0.1331*		0.8735	2.6085
2_2	Bubble P + y	kij= aij+bij/T	*0.0981*	*8.2761*	0.8427	2.6148

AspenPlus (Tc, Pc, w 값이 PRO/II와 동일하여 값이 같음)

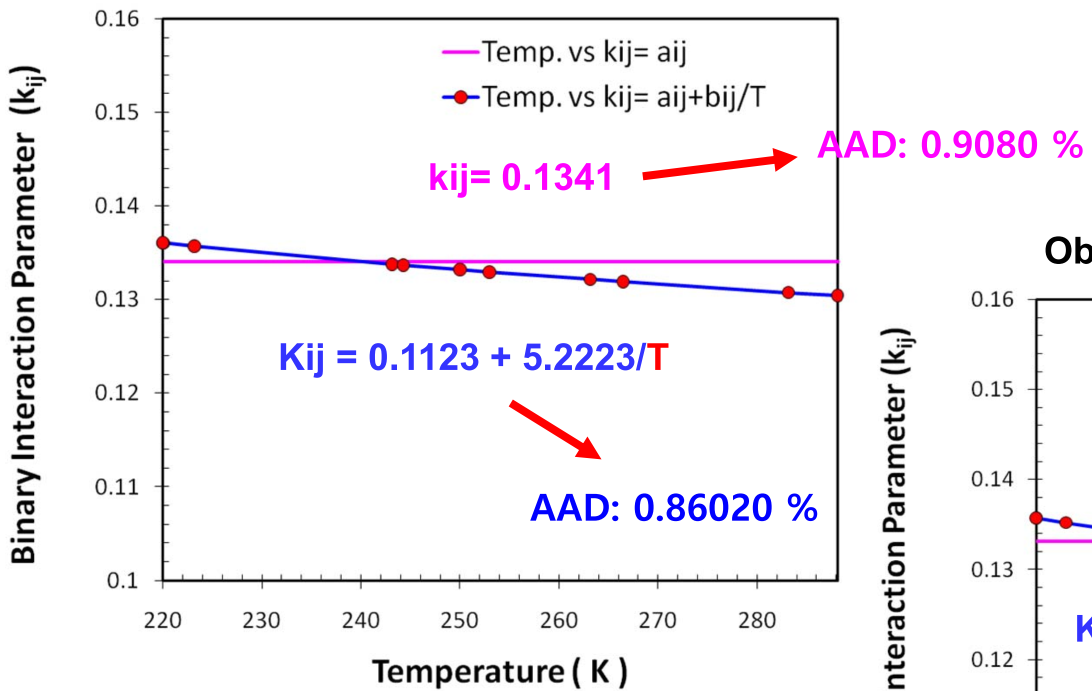
case	Object Function	BIP Mixing Rule	aij	bij	P AAD (%)	y AAD (%)
1_1	Bubble P	kij= aij	*0.1341*		0.9083	2.6029
1_2	Bubble P	kij= aij+bij/T	*0.1123*	*5.2223*	0.8602	2.6051
2_1	Bubble P + y	kij= aij	*0.1331*		0.8735	2.6085
2_2	Bubble P + y	kij= aij+bij/T	*0.0981*	*8.2761*	0.8427	2.6148

HYSYS

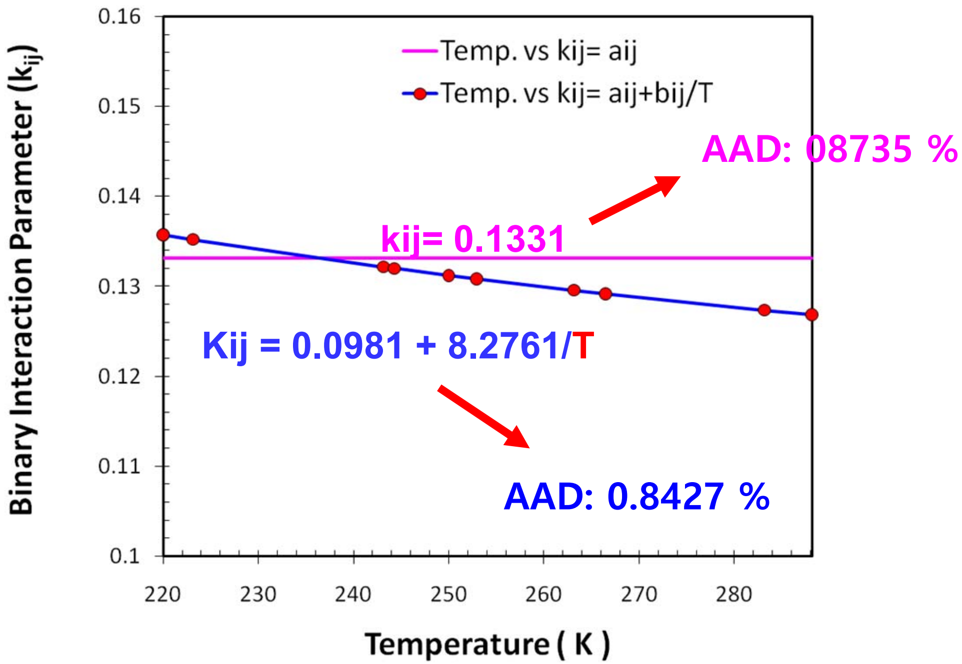
case	Object Function	BIP Mixing Rule	aij	bij	P AAD (%)	y AAD (%)
1_1	Bubble P	kij= aij	*0.1378*		0.9550	2.6618
1_2	Bubble P	kij= aij+bij/T	*0.0986*	*9.5020*	0.8530	2.6642
2_1	Bubble P + y	kij= aij	*0.1361*		0.9469	2.6688
2_2	Bubble P + y	kij= aij+bij/T	*0.0948*	*9.7124*	0.8438	2.6590

Using Tc, Pc, ω in Aspen Plus or PRO/II:

Object Function: Bubble P

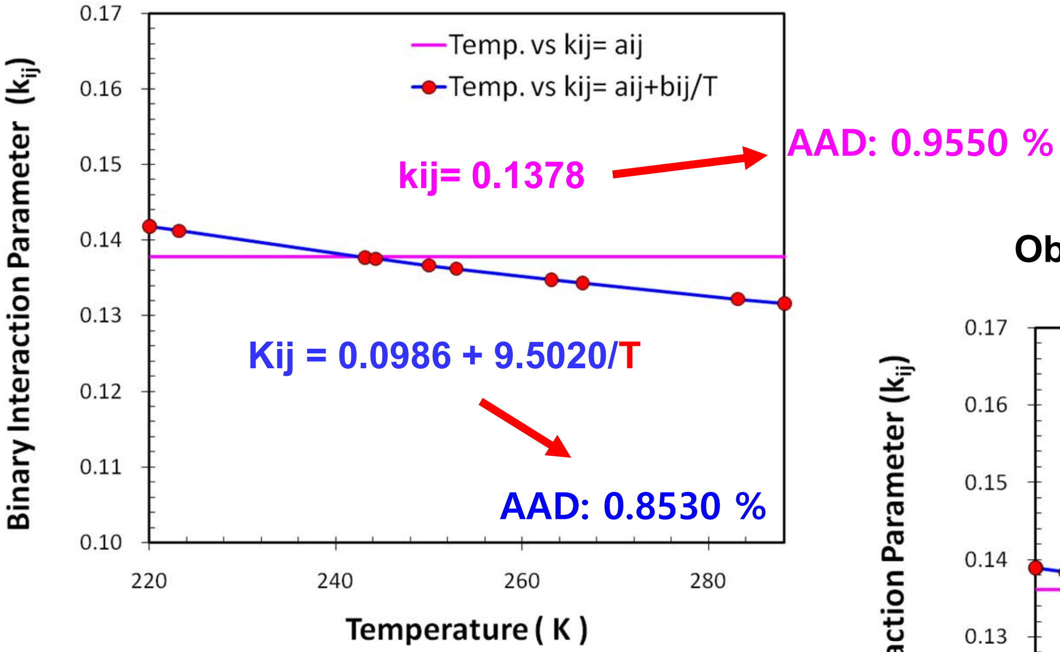


Object Function: Bubble P + y Comp.

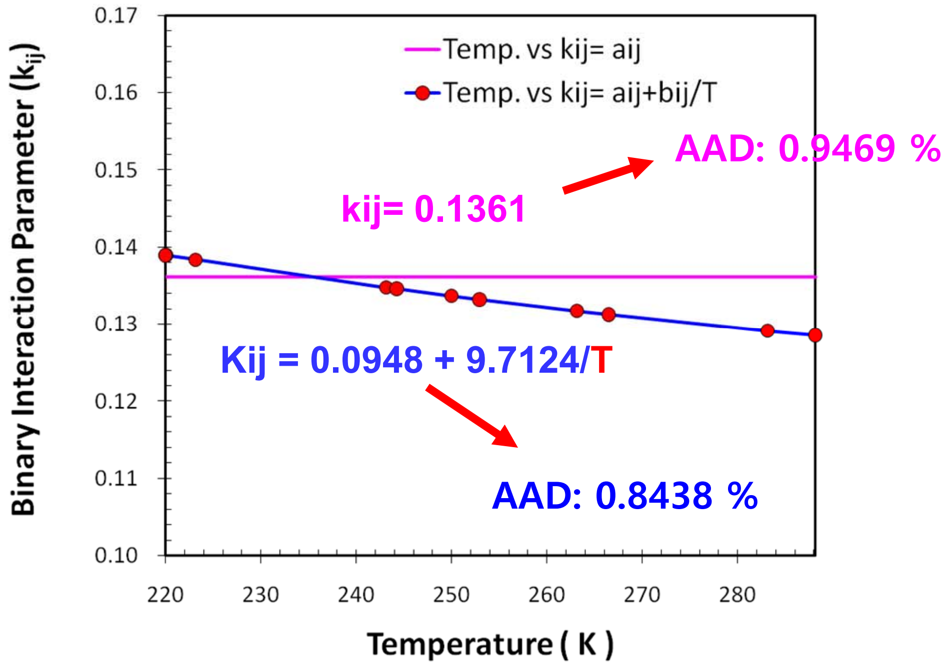


Using Tc, Pc, ω in Aspen HYSYS:

Object Function: Bubble P



Object Function: Bubble P + y Comp.



4 GERG-2008 모델식과 다른 모델식 사이의 비교

GERG-2008 Model:

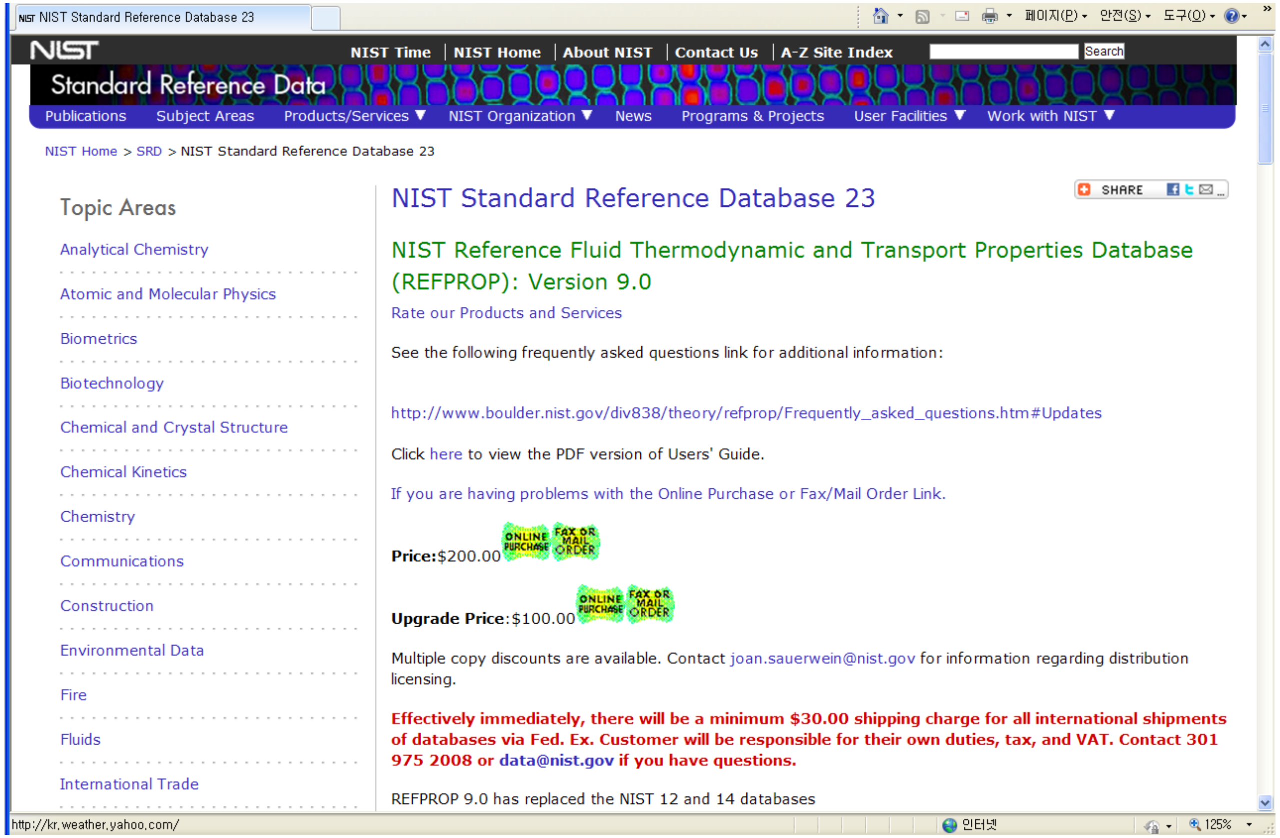
➢ GERG-2008 Equation of State

- The European Gas Research Group
- Founded in 1961
- Developed based on Wagner's EOS
- Ruhr University, Bochum, Germany

REFPROP: Physical Property DB in NIST

➢ REFPROP

- Widely used in the Refrigeration Industry
- Available from Web Site



GERG-2008:

- History of EOS in terms of Residual Helmholtz Free Energy (a^r)

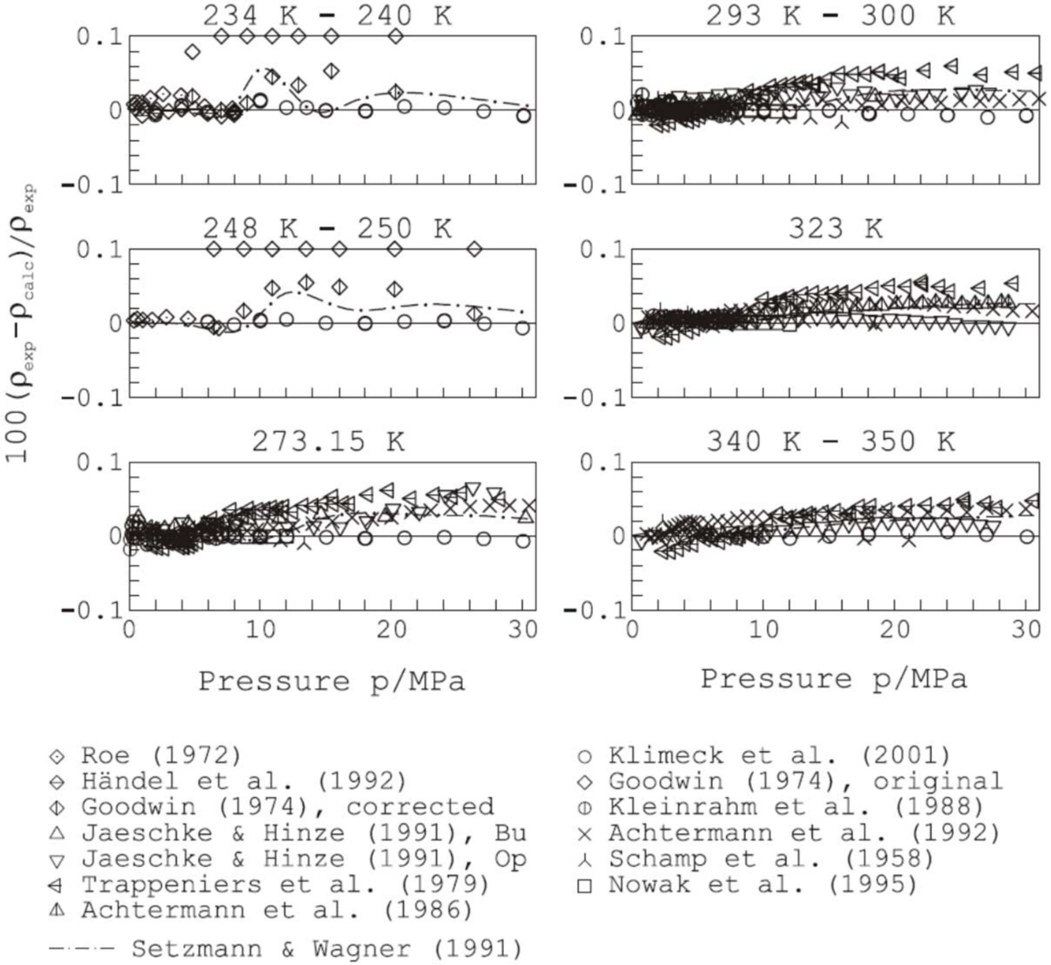
Ideal gas: $a^r = 0$

Peng-Robinson: $$\frac{a^{\mathrm{r}}}{RT} = \alpha^{\mathrm{r}}(\rho, T, \bar{x}) = \ln\left(\frac{1}{1-b\rho}\right) - \frac{a}{2\sqrt{2}\,RT}\ln\left(\frac{1+(\sqrt{2}+1)b\rho}{1-(\sqrt{2}-1)b\rho}\right)$$

Improved virial Type EOS GERG 2004:

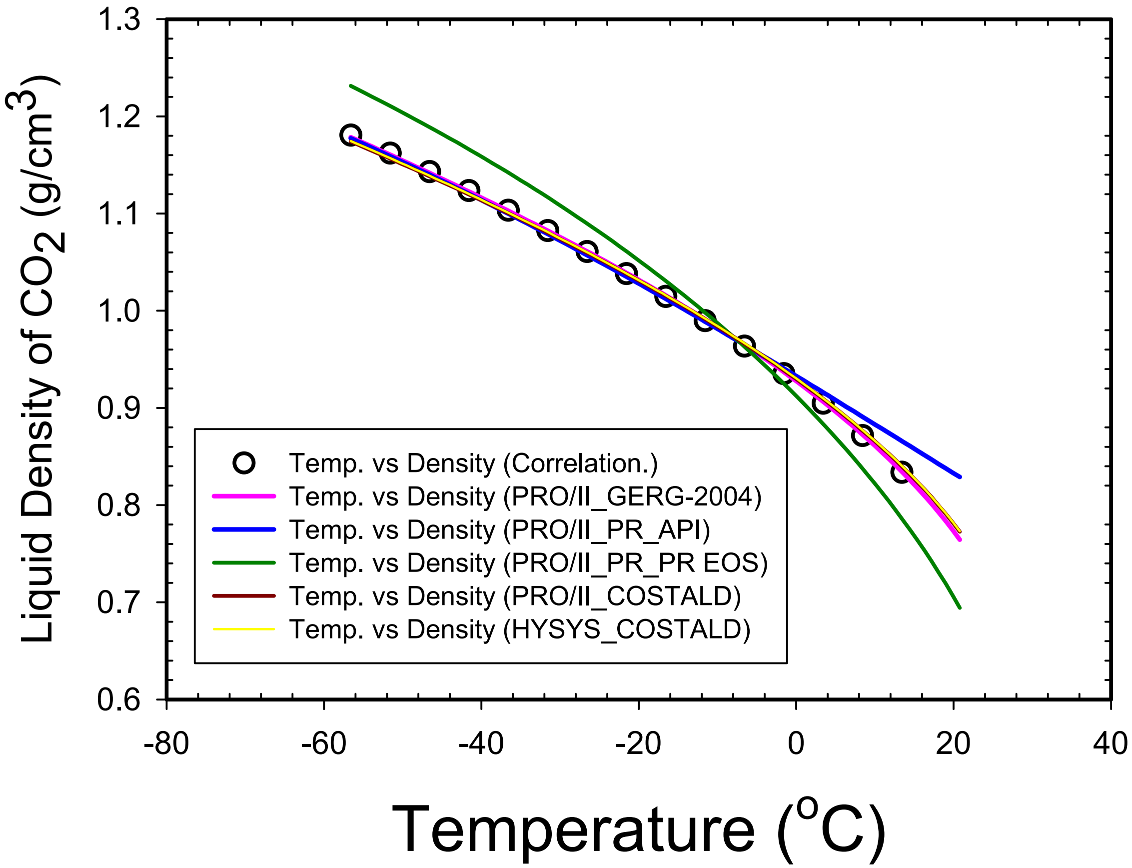
$$\alpha^{\mathrm{r}} = \sum_{k=1}^{4}\sum_{l=0}^{16} n_{kl}\,\delta^k \tau^{l/8}$$
$$+\exp(-\delta)\sum_{k=1}^{6}\sum_{l=0}^{22} n_{kl}\,\delta^k \tau^{l/8} + \exp(-\delta^2)\sum_{k=1}^{4}\sum_{l=0}^{20} n_{kl}\,\delta^k \tau^{l/4}$$
$$+\exp(-\delta^3)\sum_{k=1}^{5}\sum_{l=4}^{36} n_{kl}\,\delta^k \tau^{l/2} + \exp(-\delta^4)\sum_{k=4}^{5}\sum_{l=0}^{16} n_{kl}\,\delta^k \tau^{l}$$
$$+\exp(-\delta^5)\sum_{k=1}^{2}\sum_{l=2}^{10} n_{kl}\,\delta^{2k-1} \tau^{2l} + \exp(-\delta^6)\sum_{k=4}^{8}\sum_{l=8}^{18} n_{kl}\,\delta^k \tau^{2l}.$$

Accuracy of GERG-2008 EOS for Liquid Density:

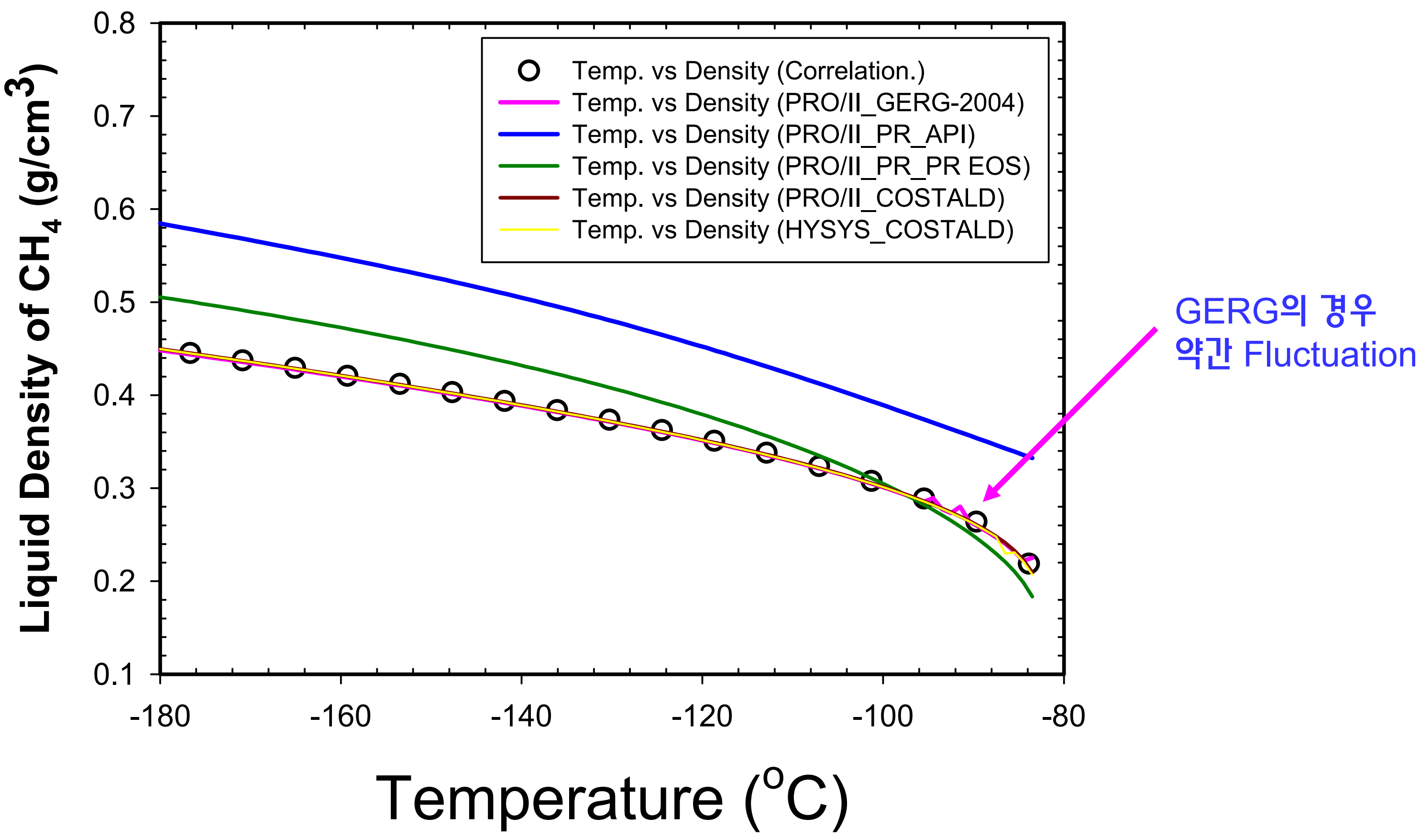


Kunz,O., R. Klimeck, W. Wagner, M. Jaeschke; „The GERG-2004 Wide-Range Equation of State for Natural Gases and Other Mixtures”, http://www.gerg.info/publications/tm/tm15_04.pdf

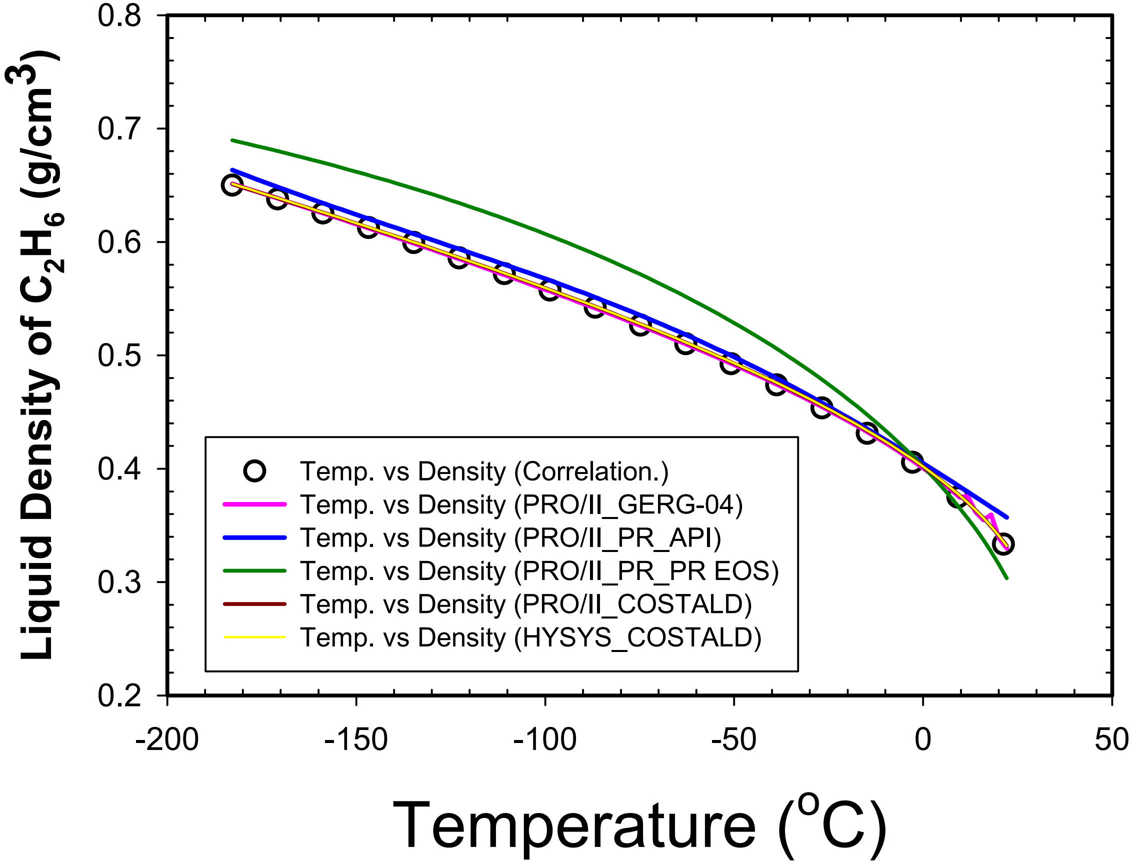
Liquid Density for Carbon Dioxide:



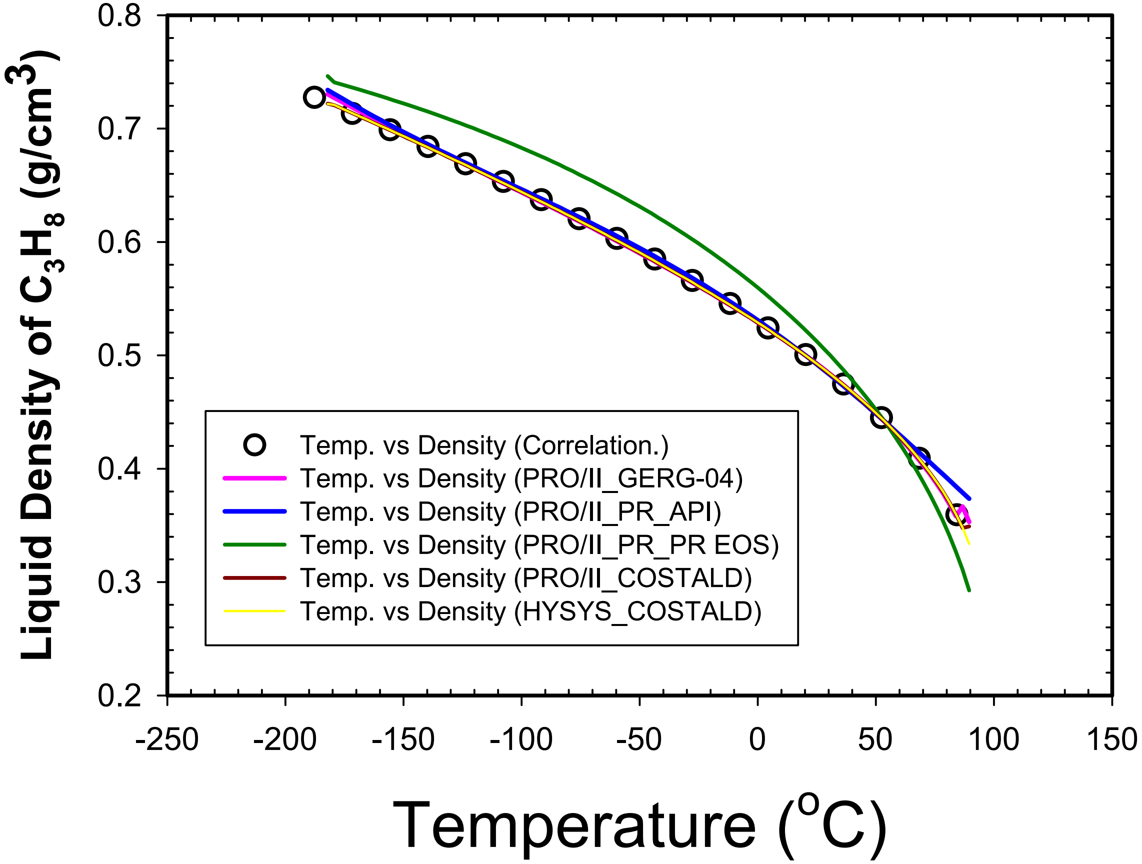
Liquid Density for Methane:



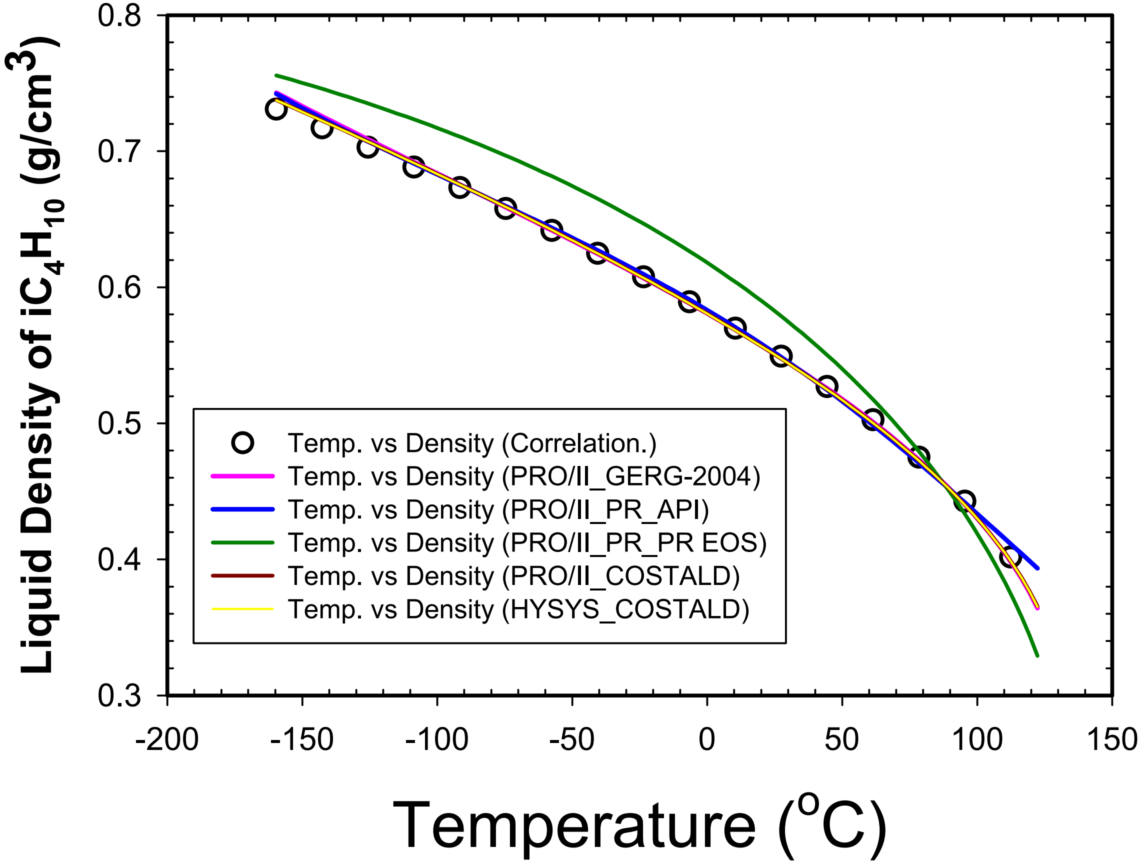
Liquid Density for Ethane:



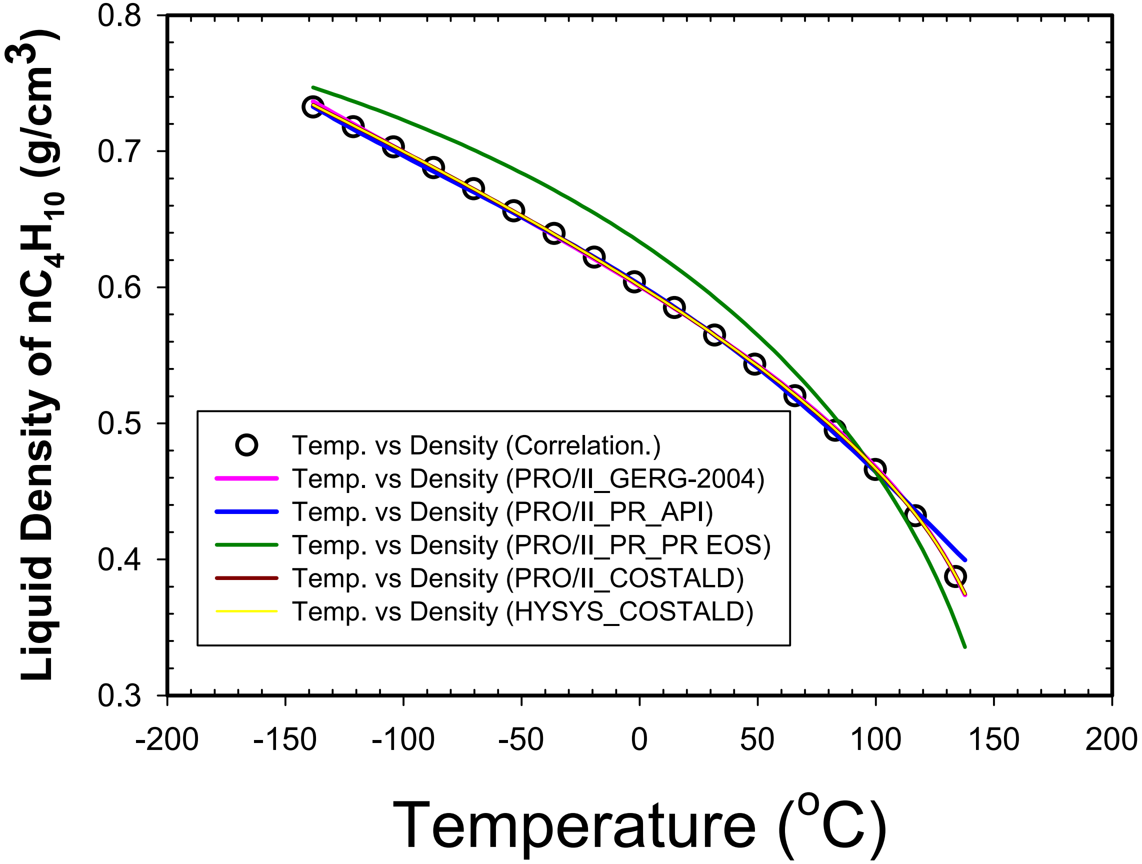
Liquid Density for Propane:



Liquid Density for Isobutane:



Liquid Density for Normal Butane:



Costald Model for LNG Liquid Density Estimation:

The corresponding-states liquid density model is suitable for prediction the liquid densities of "LNG-like" fluids. This accurate and reliable method is over 99.8% accurate in predicting the densities of light hydrocarbon mixtures.

$$V_S / V^* = V_r^{(0)} \left[1 - \omega_{SRK} V_r^{(\delta)} \right]$$

$$V_r^{(0)} = 1 + \sum_{1}^{4} A_k (1 - T_r)^{k/3}, \quad 0.25 < T_r < 0.95$$

$$V_r^{(\delta)} = \left[\sum_{0}^{3} B_k T_r^{k} \right] / \left(T_r - 1.00001 \right) \quad 0.25 < T_r < 1.0$$

GERG-2008 EOS:

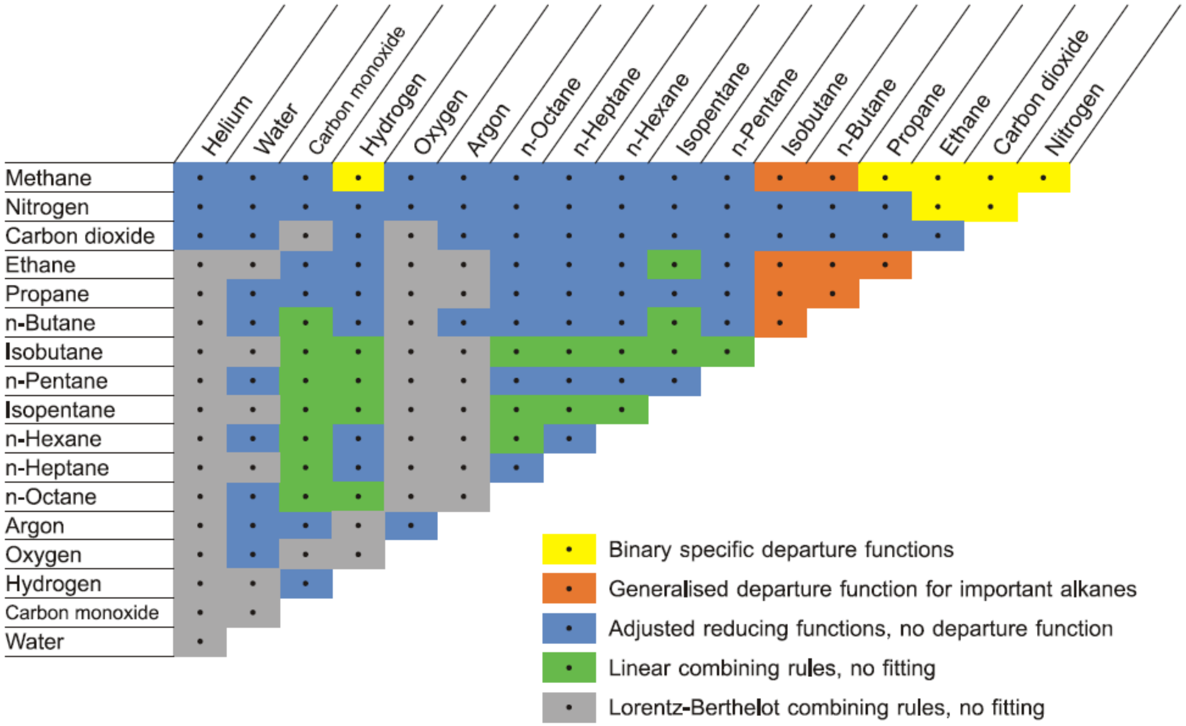
➢ Available Components

Methane	n-Butane	Hydrogen
Nitrogen	Isobutane	Oxygen
Carbon dioxide	n-Pentane	Carbon monoxide
Ethane	Isopentane	Water
Propane	n-Hexane	Helium
	n-Heptane	Argon
	n-Octane	

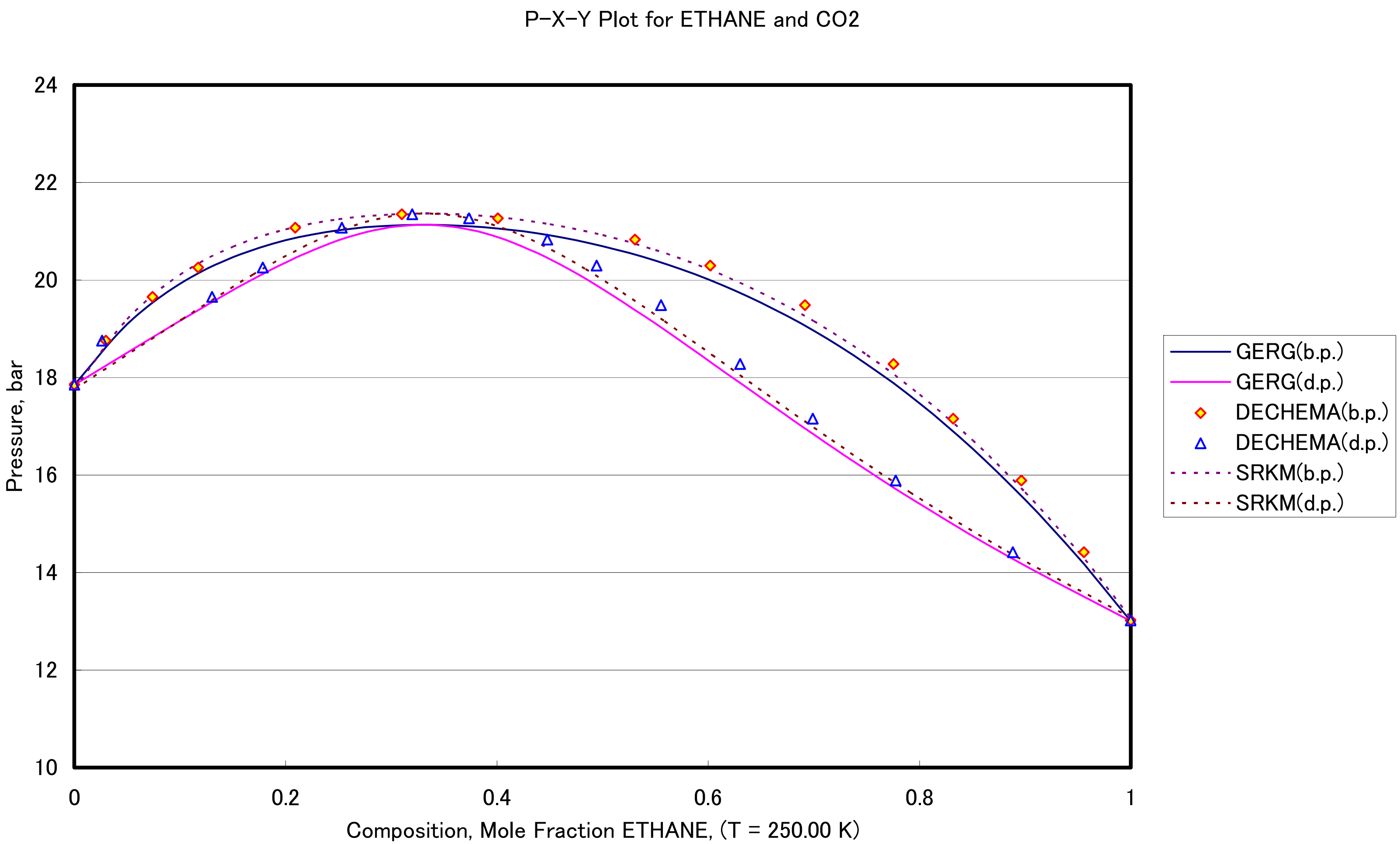
GERG-2008 EOS: Binary Interaction Parameters

➢ Binary Interaction Parameters:

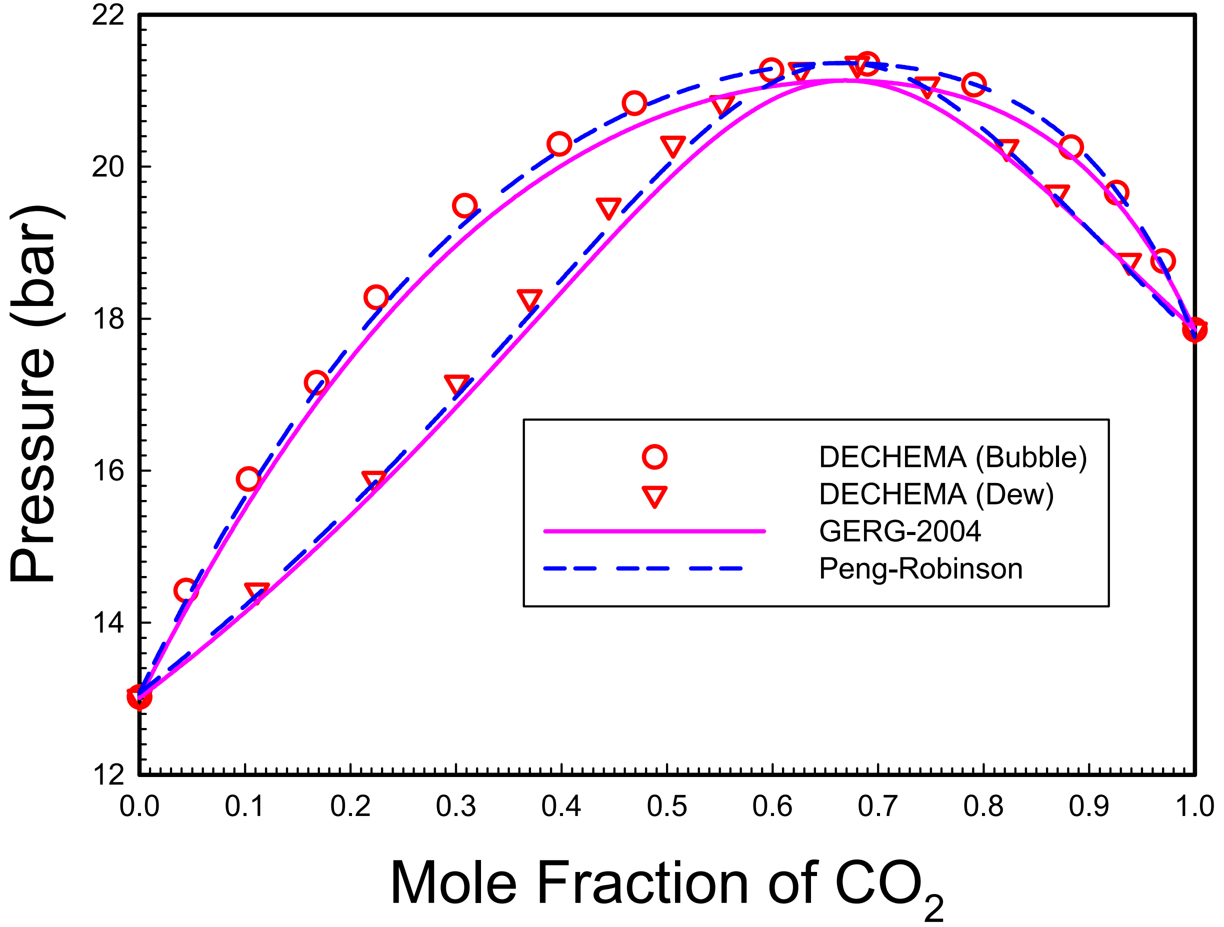
$$\alpha^{\mathrm{r}}(\delta,\tau,\bar{x}) = \sum_{i=1}^{N} x_i\, \alpha^{\mathrm{r}}_{\mathrm{o}i}(\delta,\tau) + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j F_{ij}\, \alpha^{\mathrm{r}}_{ij}(\delta,\tau),$$



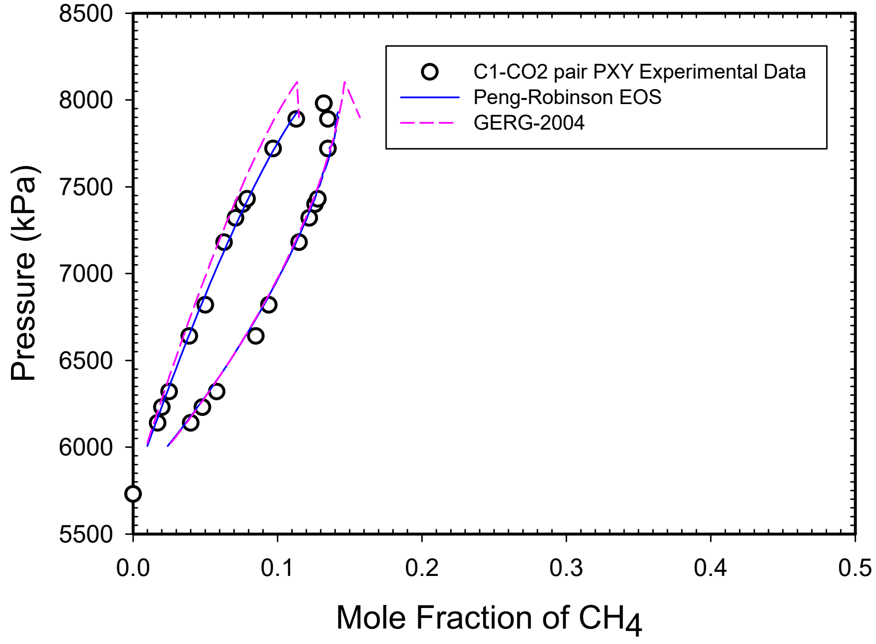
GERG is not superior to SRK in Predicting VLE:



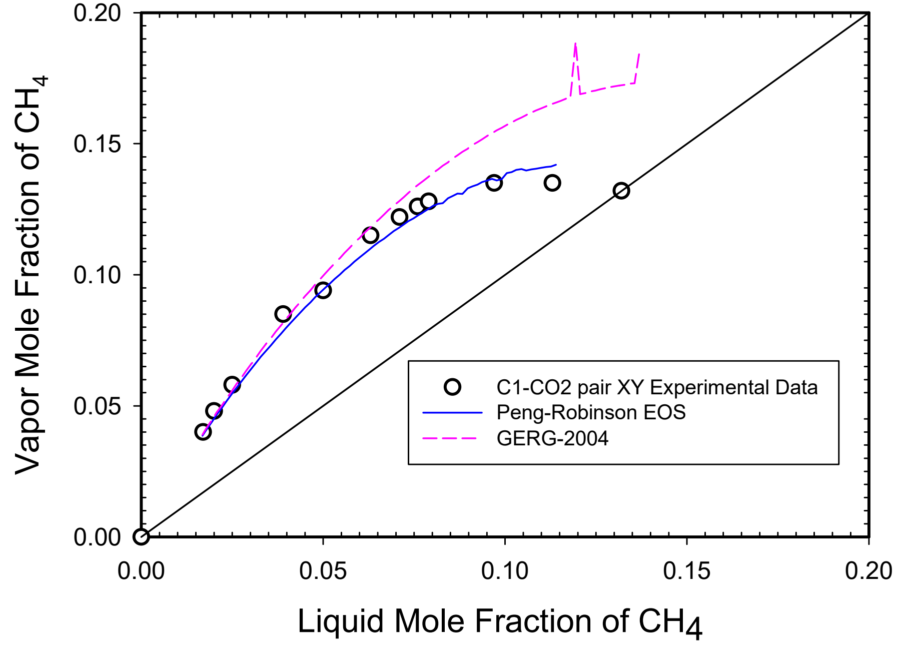
GERG is not superior to SRK in Predicting VLE:



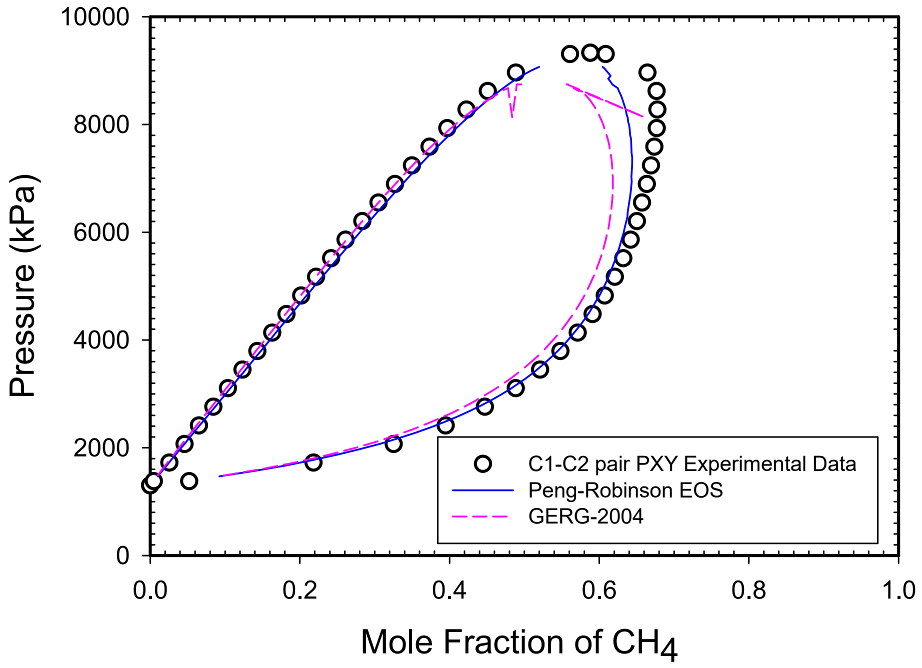
Isothermal Pxy & XY of CH_4 + CO_2 at 293.40K:



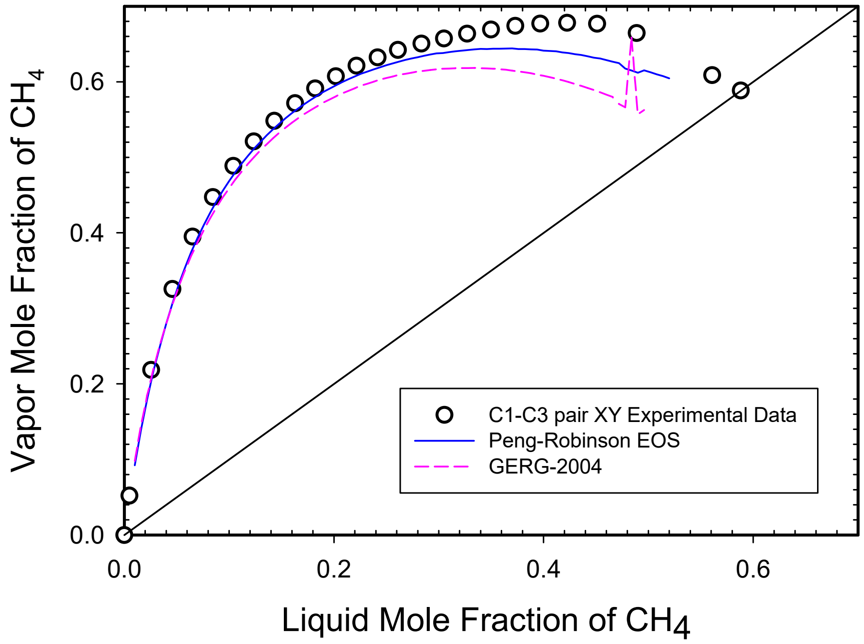
Reference: XU N.,DONG J.,WANG Y.,SHI J., FLUID PHASE EQUILIB., 81,175(1992)



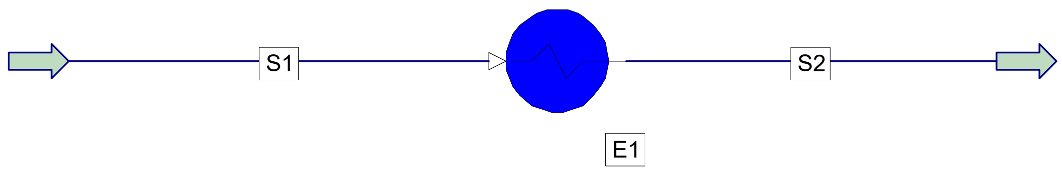
Isothermal Pxy & XY of CH_4 + C_3H_8 at 310.93K:



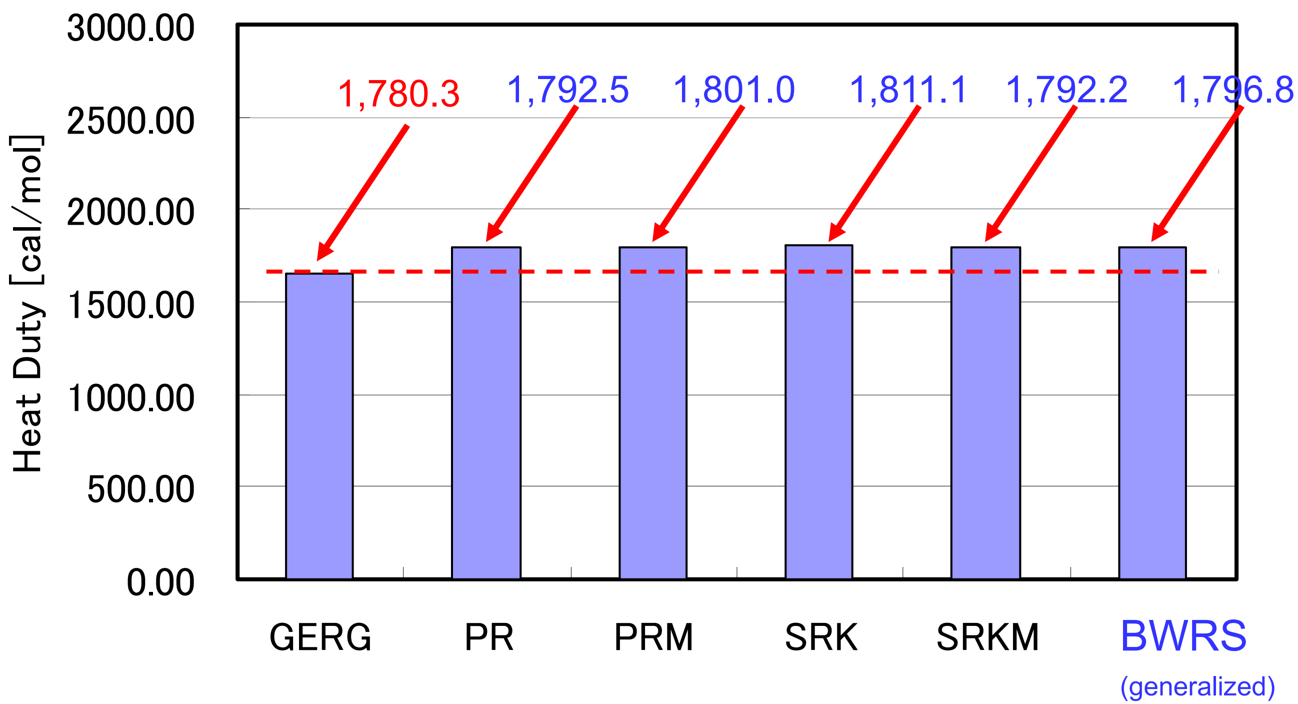
Reference: SAGE B.H.,LACEY W.N., API PROJECT, 37,THERMODYN.PROP.LIGHT.PAR./N2 (1950)



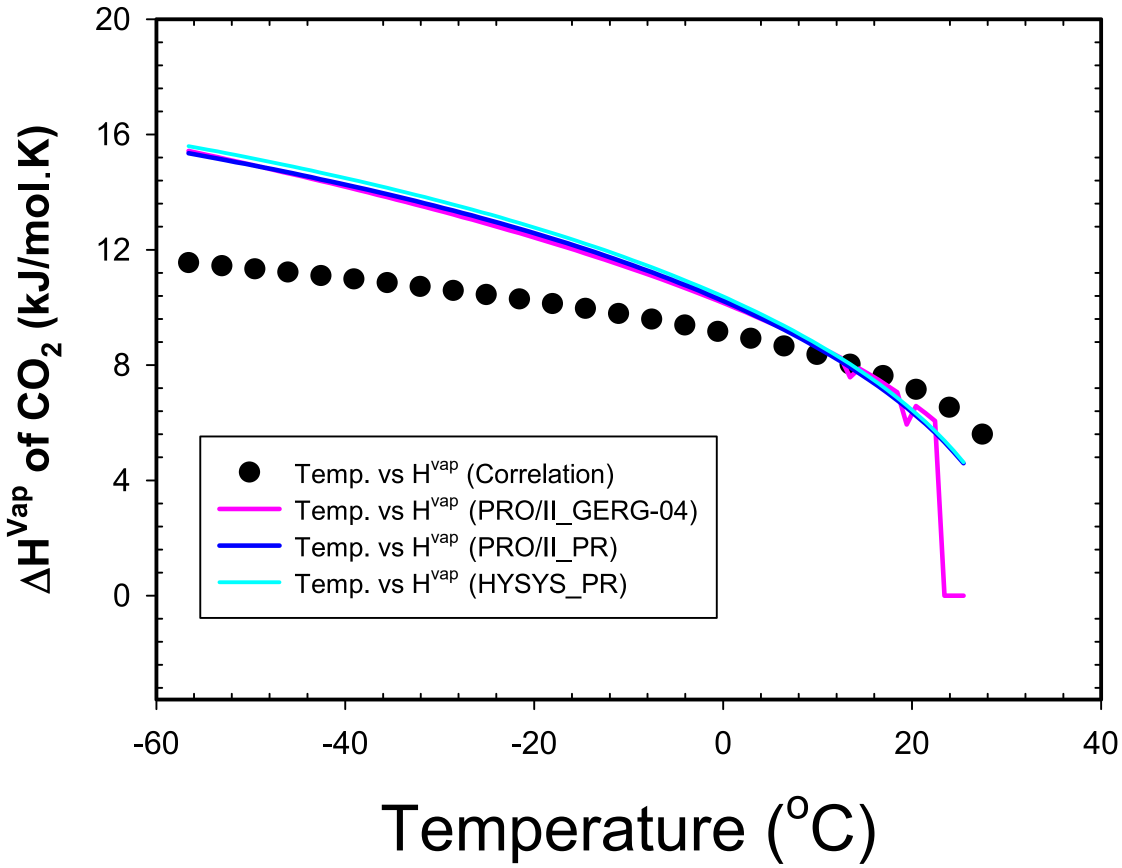
Enthalpy Prediction Example:



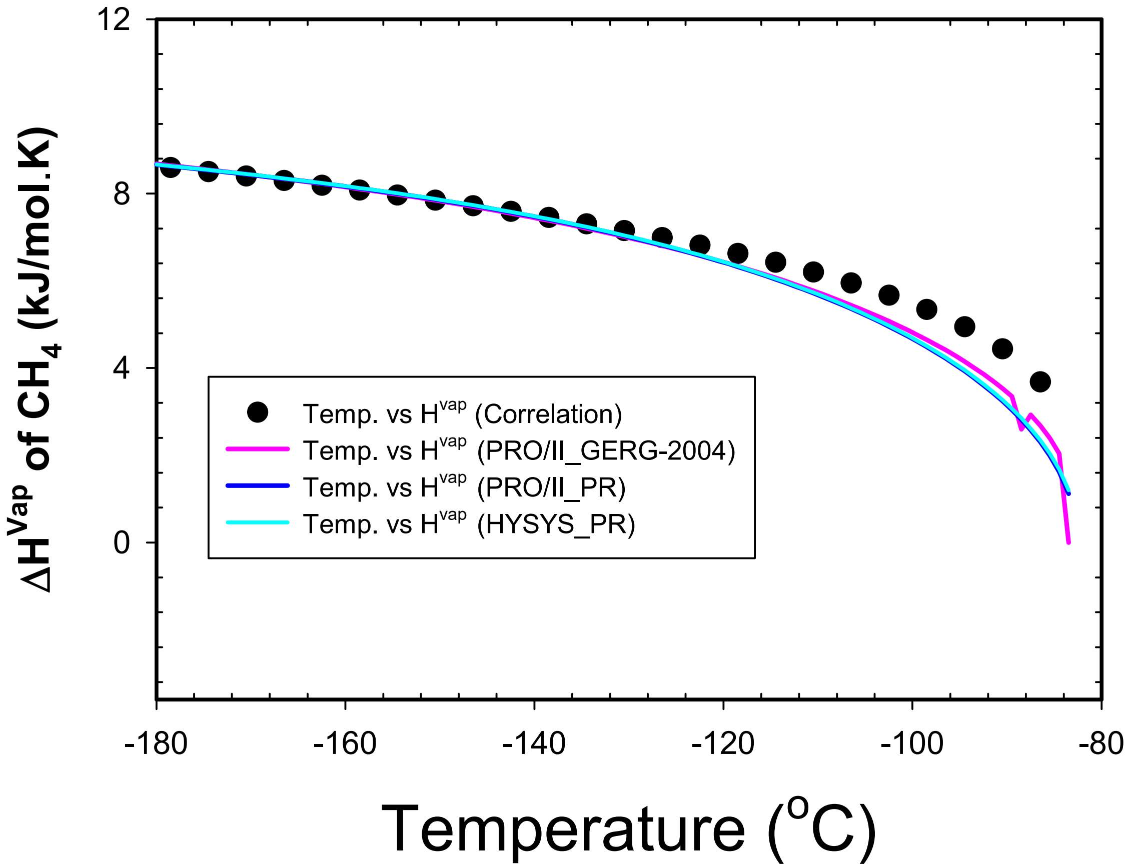
Stream Name		S1	S2
Temperature	K	253.150	313.150
Pressure	MPA	10.101	10.101
Flowrate	KG-MOL/HR	1.000	1.000



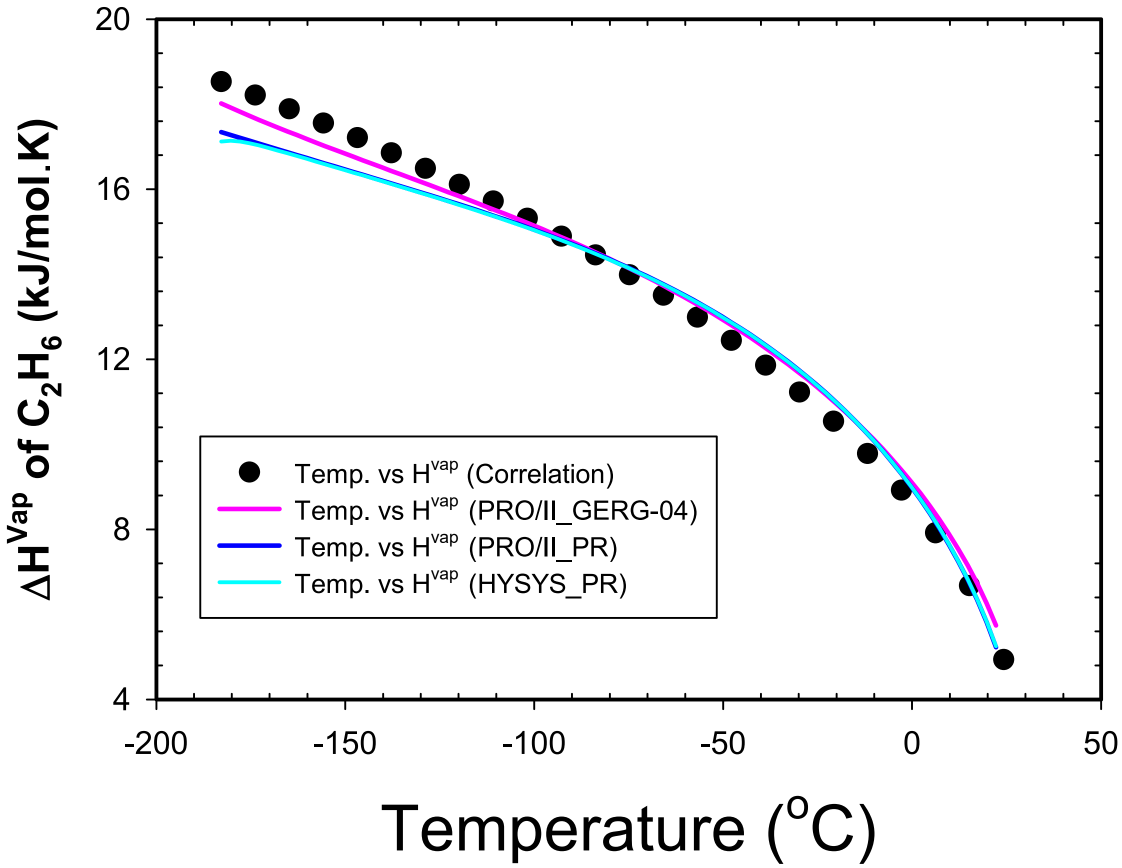
Heat of Vaporization for Carbon Dioxide:



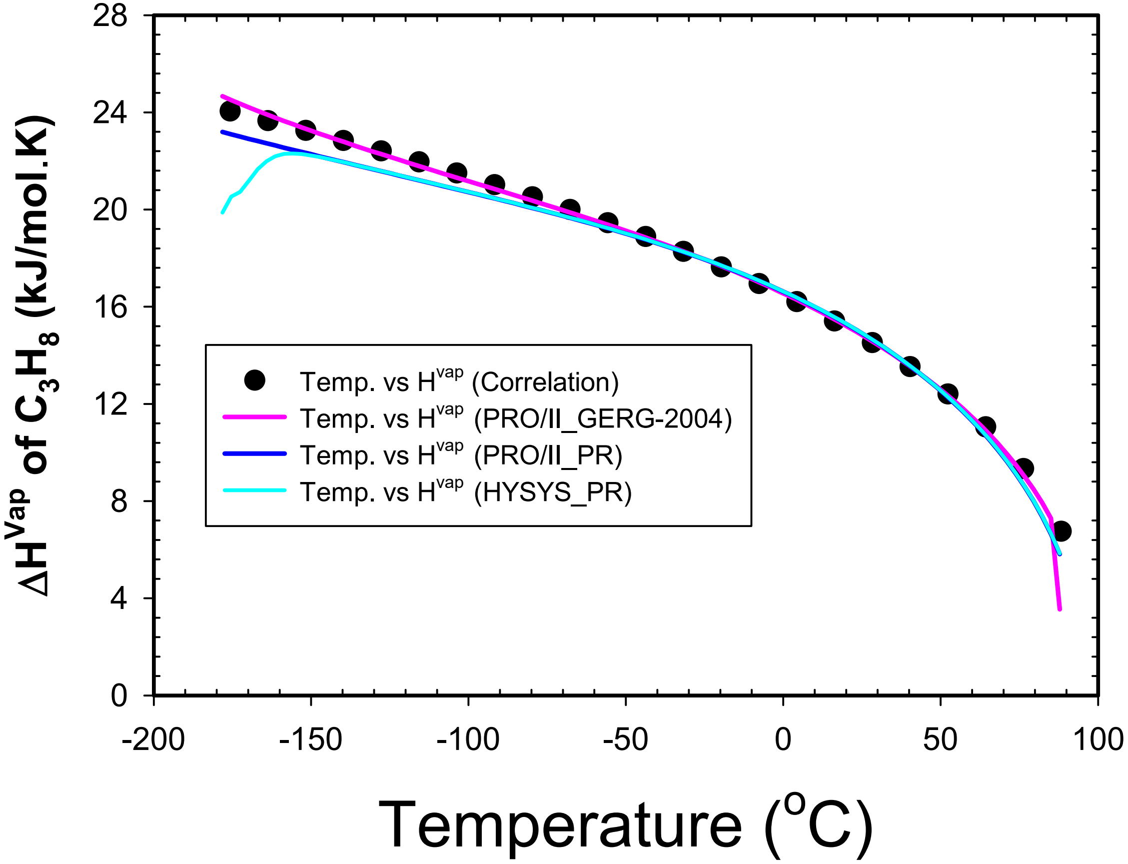
Heat of Vaporization for Methane:



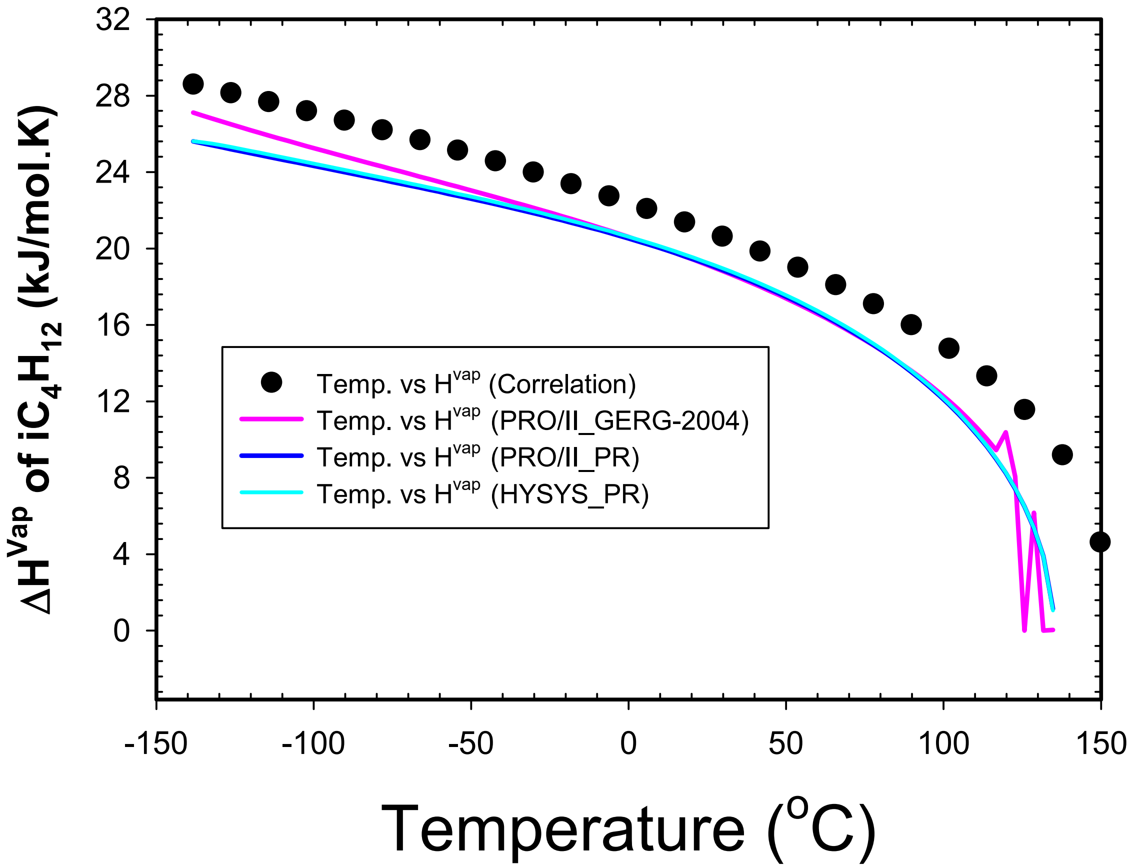
Heat of Vaporization for Carbon Ethane:



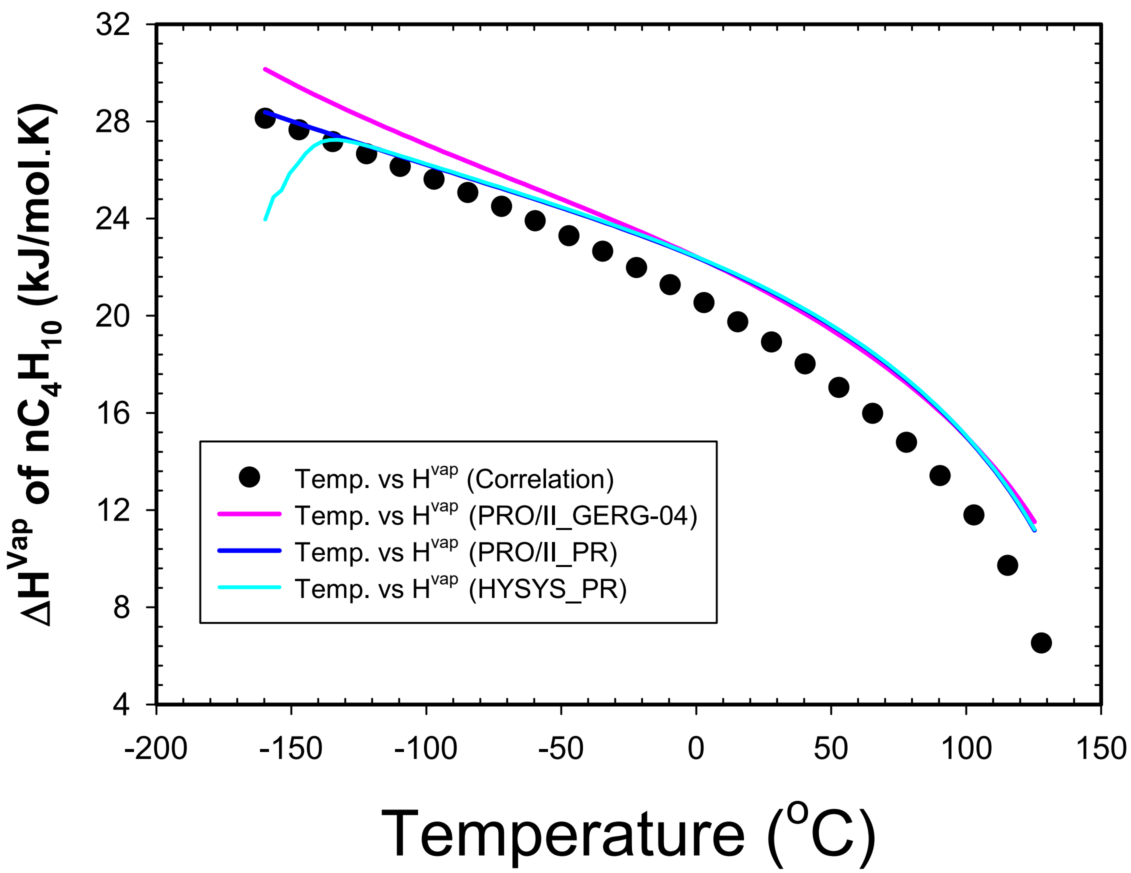
Heat of Vaporization for Propane:



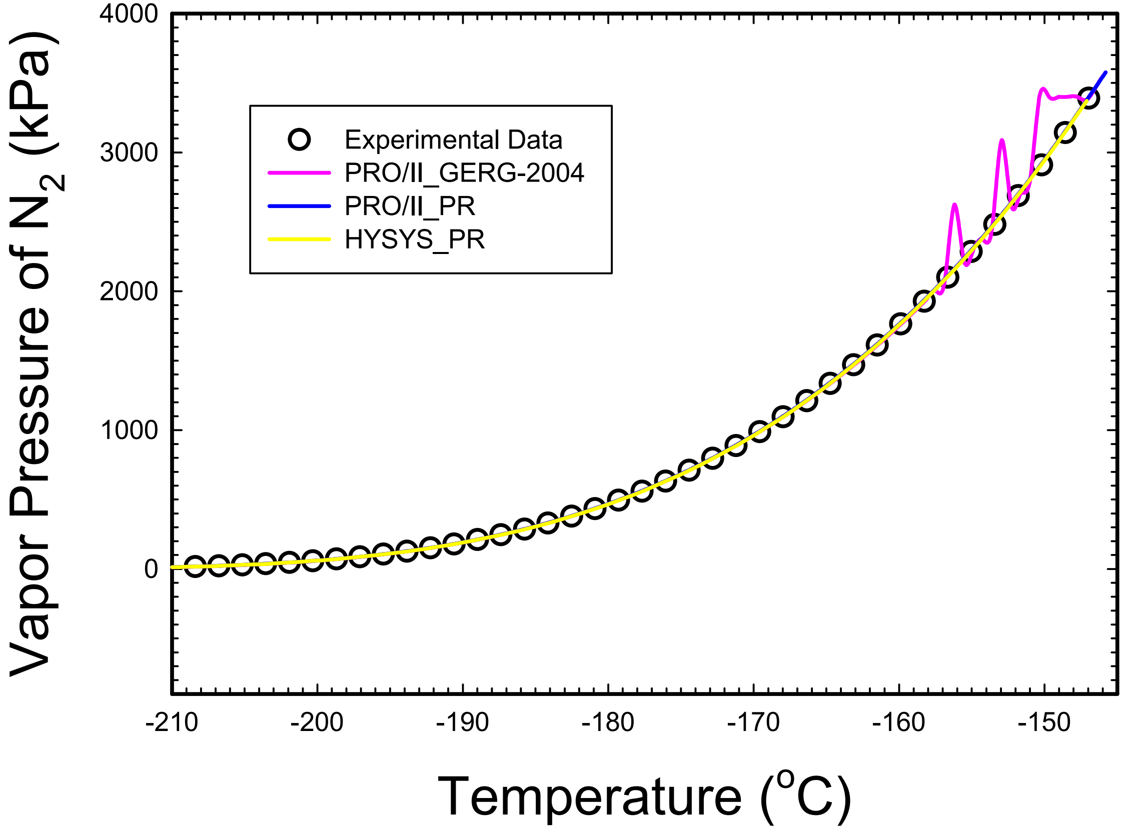
Heat of Vaporization for Isobutane:



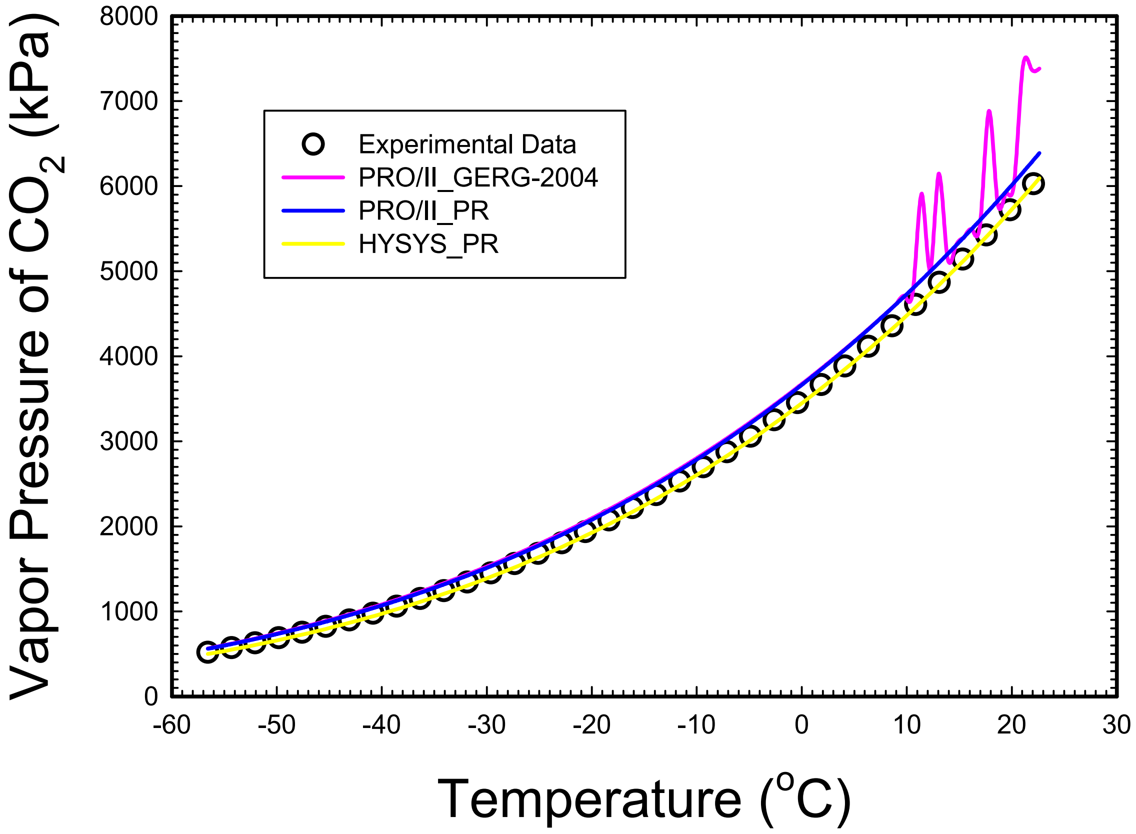
Heat of Vaporization for Normal Butane:



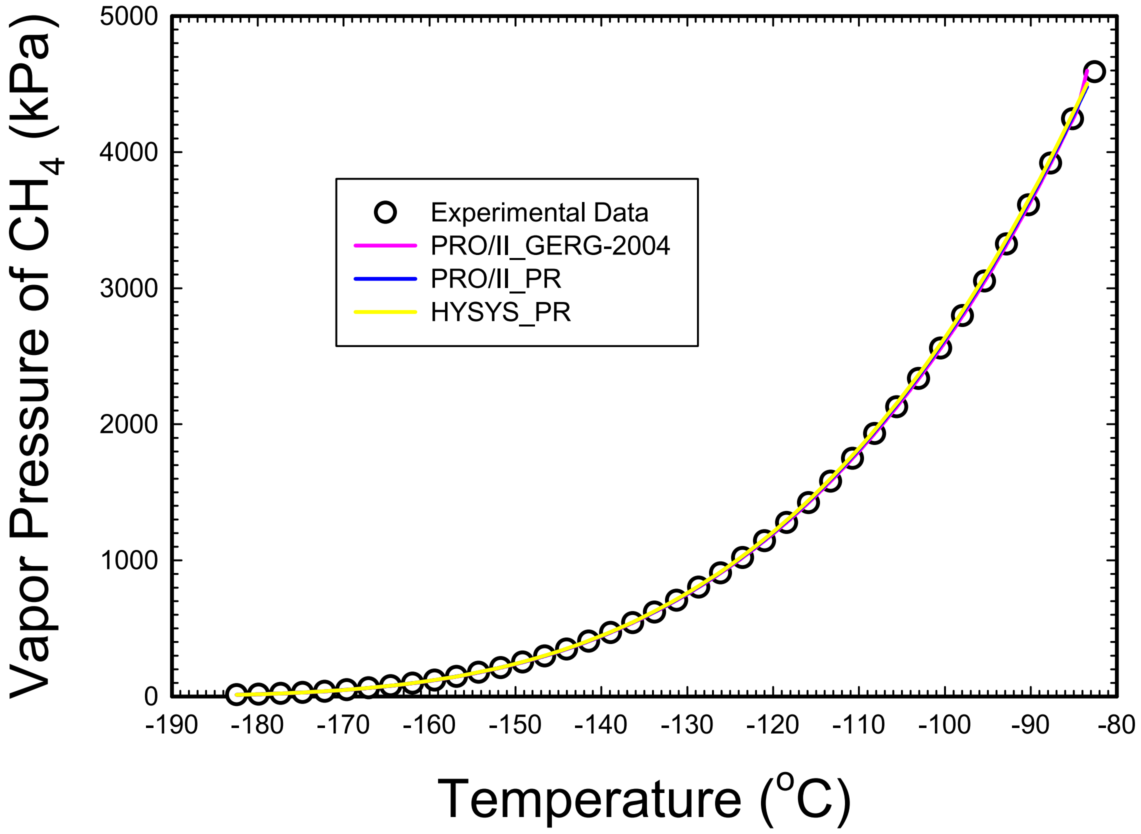
Vapor Pressure for Nitrogen:



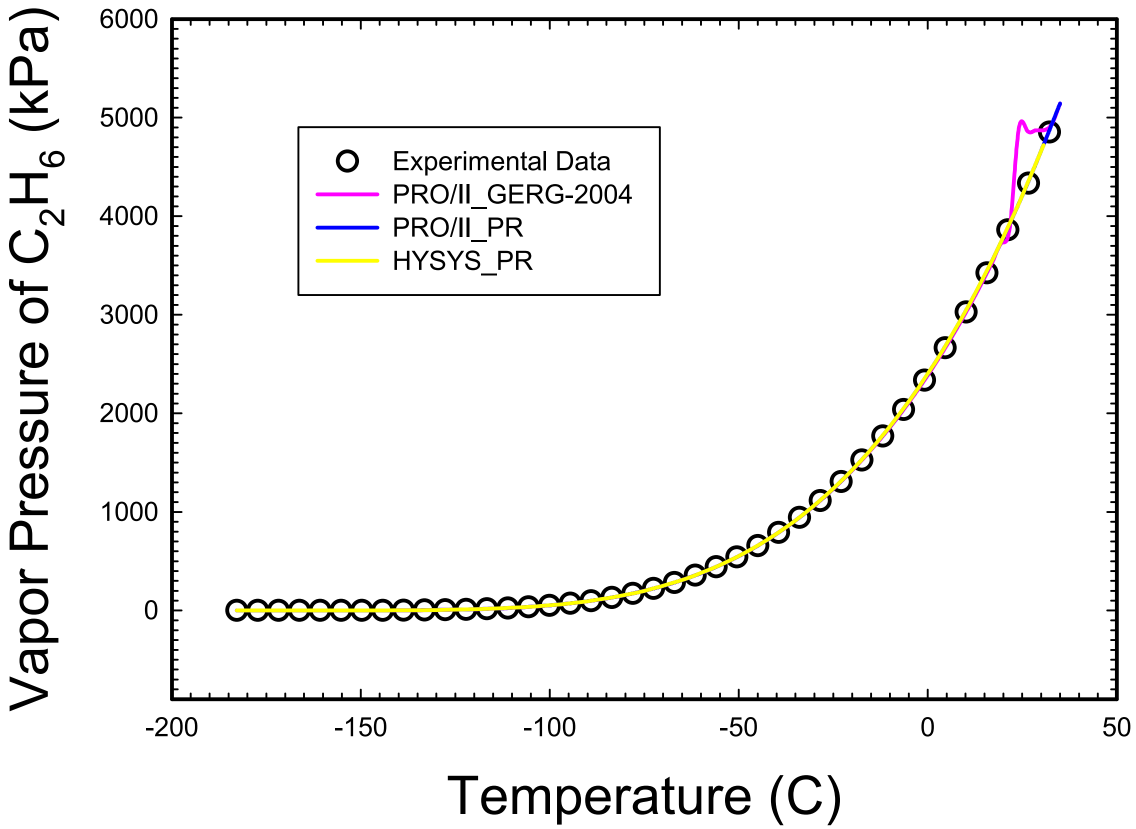
Vapor Pressure for Carbon Dioxide:



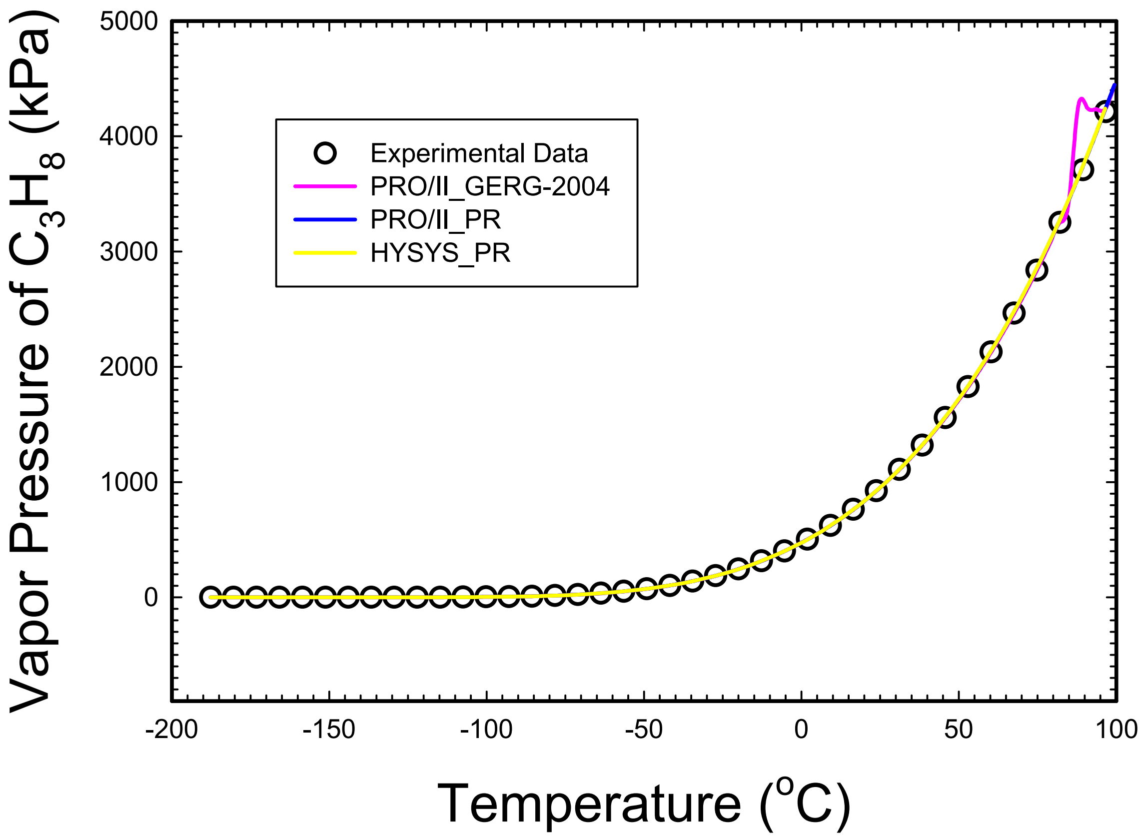
Vapor Pressure for Methane:



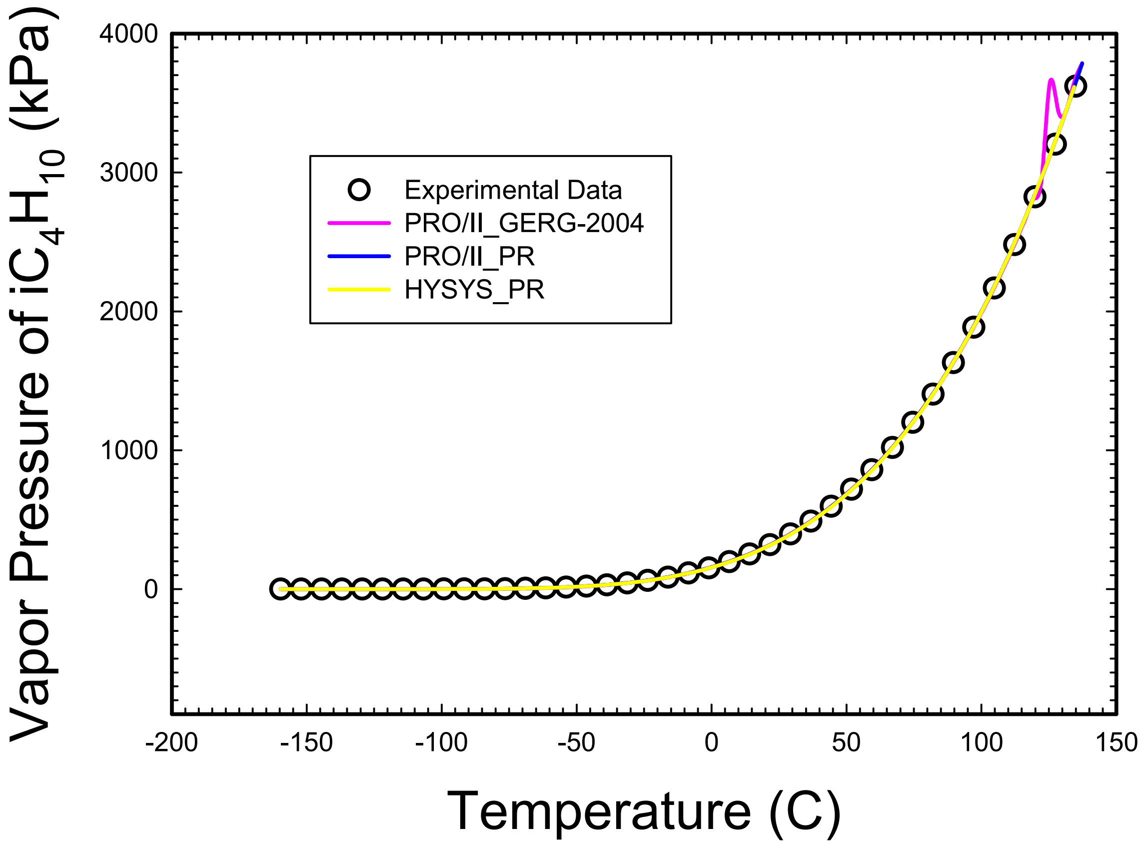
Vapor Pressure for Ethane:



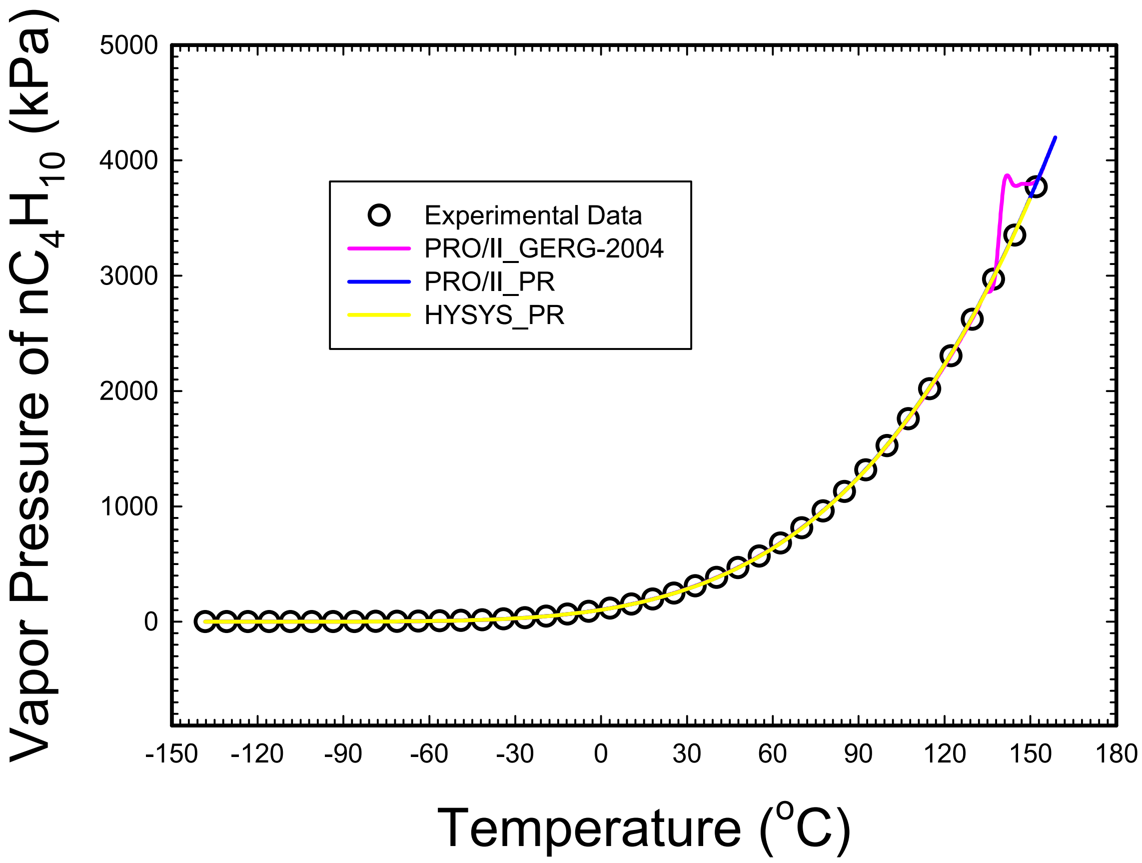
Vapor Pressure for Propane:



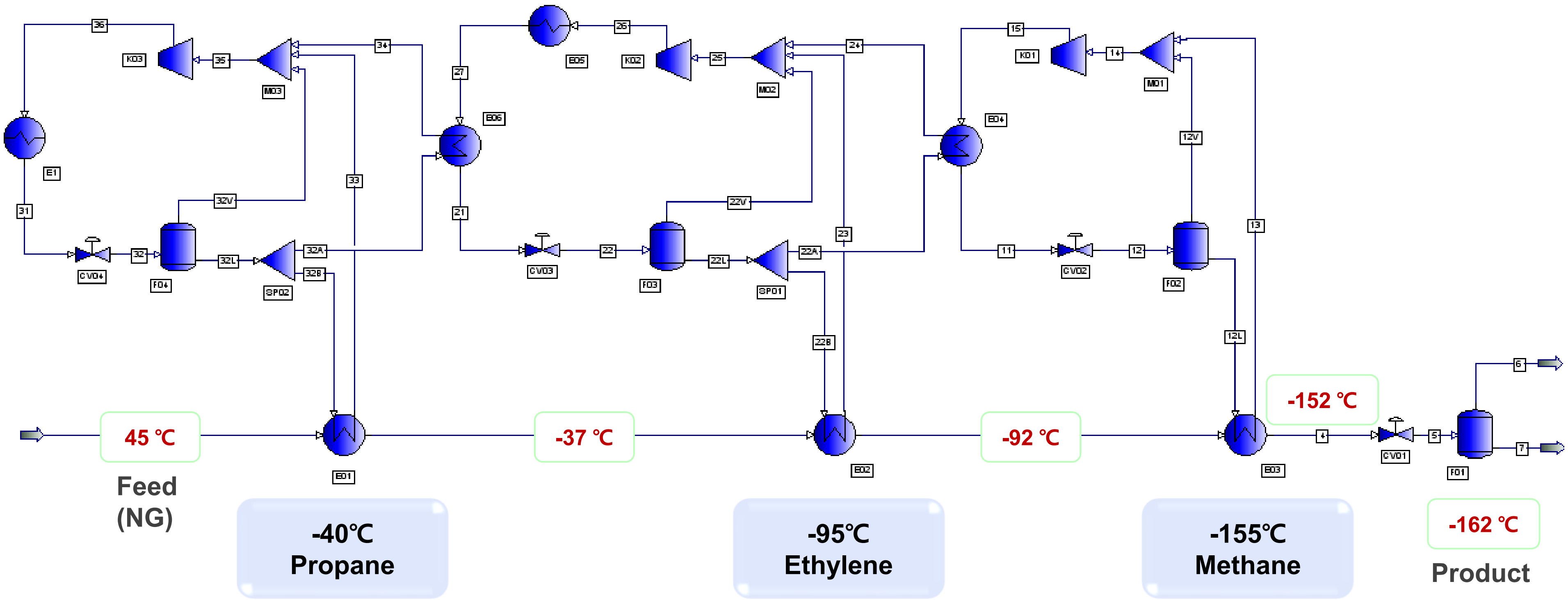
Vapor Pressure for Isobutane:



Vapor Pressure for Normal Butane:



Propane-Ethylene-Methane 냉동 사이클:



THANK YOU