BENCHMARK FLOW PROBLEMS - A ROUND-ROBIN EXERCISE

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Critical Discharge Round-Robin Exercise

For benchmarking purpose.

Thermodynamic equilibrium assumption.

Homogeneous flow (no slip).

Three inlet qualities (0.0001, 0.01, 0.1).

Case I (Cyclohexane) at 10 bara.

Case II (20% mole Ethane in n-Heptane) at 10 bara.

Case III (2.5 % mole N_2 in Cyclohexane) at 33 bara.

Proposed choked flow problems

Case	**Liquid Composition (mole)**	**P_o (bar)**	**T_o (°C)**	**x_o (vapor mass)**
Ia	100% c-C6	10	182.3	0.0001 (bubble pt)
Ib	100% c-C6	10	182.3	0.01
Ic	100% c-C6	10	182.3	0.1
IIa	20% C2/n-C7	10	51.9	0.0001 (bubble pt)
IIb	20% C2/n-C7	10	51.9	0.01
IIc	20% C2/n-C7	10	51.9	0.1
IIIa	2.5% N_2/c-C6	33	25	0.0001 (bubble pt)
IIIb	2.5% N_2/c-C6	33	25	0.01
IIIc	2.5% N_2/c-C6	33	25	0.1

Data Submission

Invite EDUG.

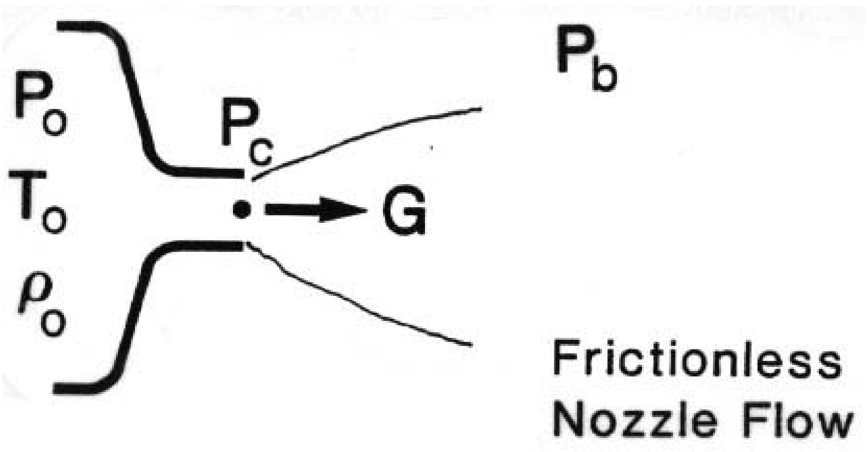
Two weeks before next US DIERS Users Group Mtg.

E-mail all relevant results (outputs) together with a summary sheet listing the mass flux G (kg/m^{2}s) and choking pressure (bar) or ratio.

Post invitation and problem specification in DIERS website.

Two-Phase Flow in Nozzle

DIERS UG San Antonio Mtg./October 20-22 2008



From Thermodynamics:

First Law (Energy Equation)

$$h_o = h + \frac{u^2}{2} = h + \frac{(Gv)^2}{2} \tag{1}$$

Second Law (Adiabatic Reversible)

$$dh = T\ dS + v\,dP \tag{2}$$

Combining:

$$G = \frac{\sqrt{2(h_o - h)}}{v} = \frac{\left[2\int_{P_o}^{P} -v\,dP\right]^{0.5}}{v} \tag{3}$$

Two-Phase Simple Fluid Expansion

$$\int \frac{dP}{\rho} \quad \text{or} \quad \int v\, dP$$

$$\frac{v}{v_o} = \omega \left(\frac{P_o}{P} - 1 \right) + 1 \qquad , \qquad \frac{\rho_o}{\rho} = \omega \left(\frac{P_o}{P} - 1 \right) + 1$$

Flashing flow (phase change):

$$\omega = \alpha_o \left(1 - 2\, \frac{P_o v_{fgo}}{h_{fgo}} \right) + \frac{C_{pf} T_o P_o}{v_o} \left(\frac{v_{fgo}}{h_{fgo}} \right)^2$$

Non – flashing flow (no phase change):

$$\omega = \frac{\alpha_o}{k}$$

Alternate Method for Multicomponent System with wide boiling pt. range (Nazario-Leung 1992 paper)

- **Use the original EOS as suggested by**

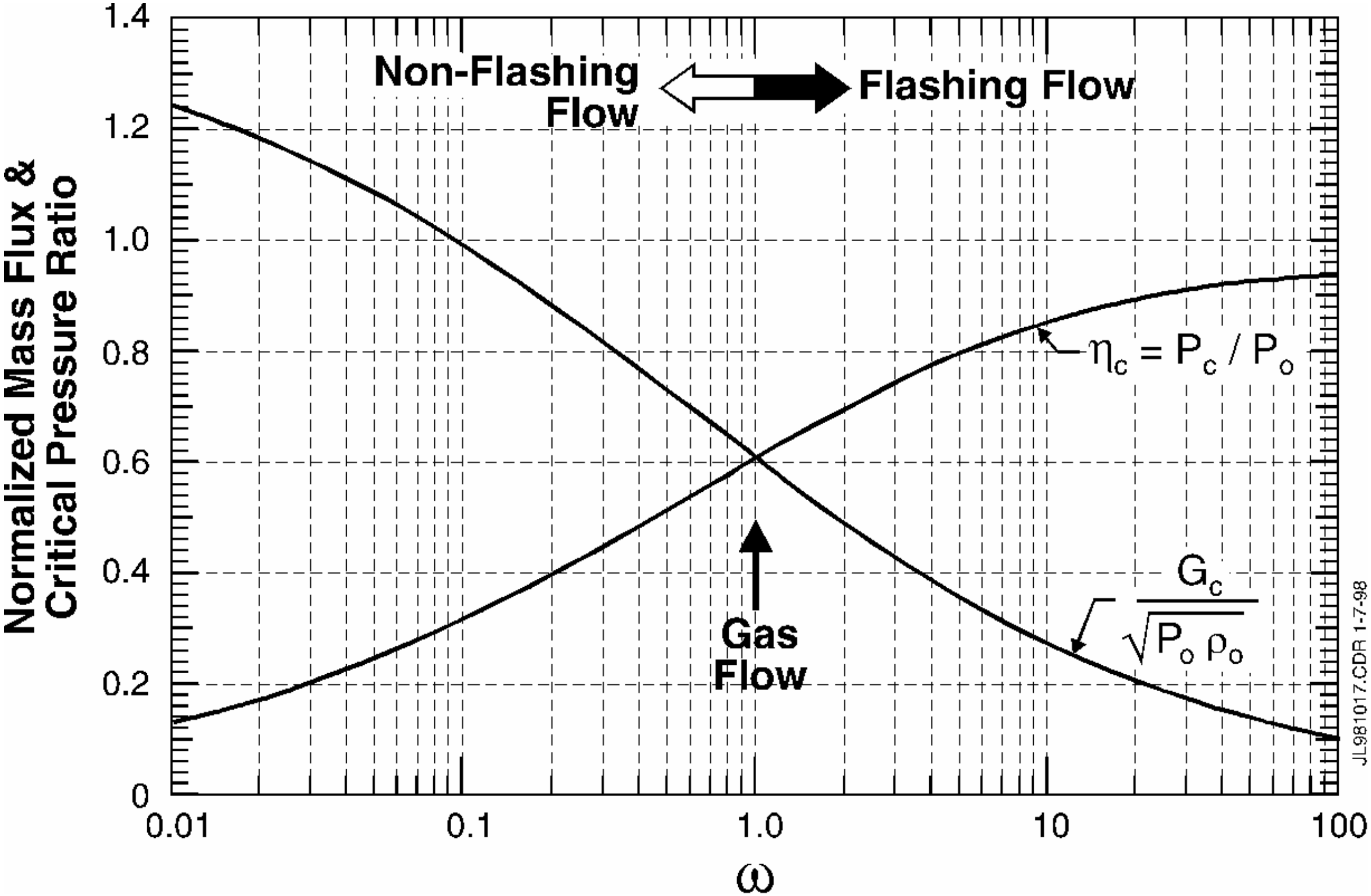
$$\frac{v}{v_o} = \omega\left(\frac{P_o}{P} - 1\right) + 1 \qquad (36)$$

- **Re-defining ω to account for realistic flashing behavior by**

$$\omega = \frac{\left(\dfrac{v}{v_o} - 1\right)}{\left(\dfrac{P_o}{P} - 1\right)} \qquad (37)$$

- **Do a multicomponent flash calculation at 90% of the inlet pressure P_o. Calculate v and ω.**

- **Use generalized G* - ω correlation to obtain the flashing flow rate per unit area.**



Flashing and non-flashing choked flow through nozzles - a unified chart. Merging the two analytical solutions, Eqs. (10) and (12). ***Source: Leung, 1990a and 1990b.***

L. L. Simpson empirical fit for P_c/P_o given by [Process Safety Progress 22(1),27(2003)]

$$P_c / P_o = \left[1 + (1.0446 - 0.0093431\,\omega^{0.5})\omega^{-0.56261}\right]^{(-0.70356 + 0.014685 \ln \omega)}$$

Participants	Flash Routine	Method of Calculation
Joseph Leung (Leung Inc.)	**in-house**	**ΔH, vdP, omega**
Greg Hendrickson (Chevron Phillips)	**Aspen Plus**	**ΔH**
James Goom (Aspen Tech.)	**Aspen Dynamics**	**ΔH, vdP (Simpson)**
Nikita Podlevskikh (CISP)	**VENT (TSS)**	$G=(dv/dP)_s^{-1/2}$
Warren Greenfield (ISP)	**SimSci PRO/II**	**ΔH**
Bob D'Alessandro (Evonik-Degussa)	**Aspen Plus**	**vdP**
Bob D'Alessandro (Evonik-Degussa)	**SuperChem**	**vdP**
Harold Fisher (Fisher Inc.)	**Proprietary**	**vdP (Simpson)**
Georges Melhem (Iomosaic)	**SuperChem**	**vdP**
Enio Kumpinsky (Ashland)	**SuperChem**	**vdP**
Dan Smith (Albermarle)	**in-house**	**vdP (Simpson)**
	in-house	**omega 0.9**
	Chemcad	**unknown**

100% c-C6, 10 bar, 182.3°C

Method (initials)	**Case Ia x_o = 0.0001**		**Case Ib x_o = 0.01**		**Case Ic x_o = 0.1**	
	G_c (kg/m²s)	**η_c**	**G_c (kg/m²s)**	**η_c**	**G_c (kg/m²s)**	**η_c**
ω_o (JL)	6140	0.863	6020	0.849	5190	0.778
$\omega_{0.9}$ (JL)	6160	0.863	6020	0.849	5210	0.777
vdP (JL)	6120	0.870	5990	0.857	5180	0.780
Aspen ΔH (GH)	5940	0.845	5810	0.835	5100	0.794
Aspen ΔH (JG)	6050	0.863	5930	0.850	5160	0.778
Aspen vdP (JG)	6090	0.864	5960	0.852	5170	0.780
Vent (NP)	6150	0.867	6010	0.853	5200	0.795
Simsci ΔH (WG)	6050	0.860	NA	NA	NA	NA
Aspen vdP (RD)	6130	0.870	5980	0.860	5120	0.790
SuperChem vdP (RD)	6060	0.875	5920	0.866	5100	0.784
SuperChem vdP (GH)	6080	0.875	5980	0.866	5160	0.784
vdP (HF)	5850	0.873	5720	0.862	4940	0.793
Mean Value	**6070**	**0.866**	**5940**	**0.854**	**5140**	**0.785**
Std. Dev.	**90**	**0.008**	**70**	**0.009**	**80**	**0.007**

20% C2/n-C7 (Liq. Comp.), 10 bar, 51.9°C

Method (initials)	**Case IIa x_o = 0.0001**		**Case IIb x_o = 0.01**		**Case IIc x_o = 0.1**	
	G_c (kg/m²s)	**η_c**	**G_c (kg/m²s)**	**η_c**	**G_c (kg/m²s)**	**η_c**
$\omega_{0.9}$ (JL)	9850	0.762	8940	0.733	5650	0.652
vdP (JL)	9780	0.768	8890	0.738	5650	0.650
Aspen ΔH (GH)	9700	0.783	8800	0.731	5600	0.659
Aspen ΔH (JG)	9800	0.762	8910	0.733	5650	0.651
Aspen vdP (JG)	9810	0.761	8910	0.732	5650	0.648
Vent (NP)	9180	0.750	8500	0.717	5670	0.640
Simsci ΔH (WG)	9870	0.755	NA	NA	NA	NA
Aspen vdP (RD)	9920	0.760	8970	0.730	5680	0.650
SuperChem vdP (RD)	9910	0.757	8950	0.731	5650	0.653
SuperChem vdP (GH)	9970	0.750	9040	0.725	5700	0.651
vdP (HG)	9840	0.756	8880	0.730	5510	0.656
Mean Value	**9780**	**0.760**	**8880**	**0.730**	**5640**	**0.651**
Std. Dev.	**210**	**0.009**	**150**	**0.006**	**50**	**0.005**

2.5% N_2/c-C6 (Liq. Comp.), 33 bar, 25°C

Method (initials)	**Case IIIa x_o = 0.0001**		**Case IIIb x_o = 0.01**		**Case IIIc x_o = 0.1**	
	G_c (kg/m²s)	**η_c**	**G_c (kg/m²s)**	**η_c**	**G_c (kg/m²s)**	**η_c**
$\omega_{0.9}$ (JL)	47190	0.377	38050	0.456	19630	0.567
vdP (JL)	46600	0.390	37800	0.460	19630	0.566
Aspen ΔH (GH)	45000	0.382	37000	0.458	19550	0.565
Aspen ΔH (JG)	43880	0.377	36090	0.453	20060	0.566
Aspen vdP (JG)	43620	0.377	35970	0.449	20190	0.560
Vent (NP)	44800	0.355	40730	0.403	22040	0.494
Simsci ΔH (WG)	44990	0.385	NA	NA	NA	NA
Aspen vdP (RD)	45900	0.382	37390	0.455	19410	0.567
SuperChem (GM)	45850	0.378	37430	0.464	19330	0.567
SuperChem (GH)	46570	0.387	37440	0.462	19650	0.568
vdP (HF)	45880	0.382	37470	0.458	19390	0.570
Mean	**45480**	**0.379**	**37540**	**0.452**	**19890**	**0.559**
Std. Dev.	**1130**	**0.009**	**1310**	**0.018**	**810**	**0.023**

20% C2/n-C7 (Liq. Comp.), 10 bar, 51.9°C

Sensitivity to VLE model, ΔH, vdP (Aspen)

Method (initials)	**Case IIIa x_o = 0.0001**		**Case IIIb x_o = 0.01**		**Case IIIc x_o = 0.1**	
	G_c (kg/m²s)	**η_c**	**G_c (kg/m²s)**	**η_c**	**G_c (kg/m²s)**	**η_c**
Aspen ΔH , kij = 0.0067 (JG)	9800	0.762	8910	0.733	5650	0.651
Aspen vdP, kij = 0.0067 (JG)	9810	0.761	8910	0.732	5650	0.648
Mean Value	9780	0.760	8880	0.730	5640	0.651
Std. Dev.	210	0.009	150	0.006	50	0.005

2.5% N_2/c-C6 (Liq. Comp.), 33 bar, 25°C

Sensitivity to VLE model (Aspen)

Method (initials)	**Case IIIa x_o = 0.0001**		**Case IIIb x_o = 0.01**		**Case IIIc x_o = 0.1**	
	G_c (kg/m²s)	**η_c**	**G_c (kg/m²s)**	**η_c**	**G_c (kg/m²s)**	**η_c**
Aspen ΔH , NRTL (JG)	43880	0.377	36090	0.453	20060	0.566
Aspen vdP, NRTL (JG)	43620	0.377	35970	0.449	20190	0.560
Aspen ΔH , kij=0.176 (JG)	43970	0.375	36080	0.452	19950	0.566
Aspen ΔH , kij= (GH)	45000	0.382	37000	0.458	19550	0.565
Mean (ALL submitted)	45480	0.379	37540	0.452	19890	0.559
Std. Dev. (All submitted)	1130	0.009	1310	0.018	810	0.023

Sensitivity to liquid density for bubble pt mass flux evaluation

Method (initials)	**Case Ia $x_o = 0.0001$ Cyclo-C6**		**Case IIa $x_o = 0.0001$ C2-nC7**		**Case IIIa $x_o = 0.0001$ N2-cycloC6**	
	Liquid density (kg/m^3)	**G_c (kg/m^2s)**	**Liquid density (kg/m^3)**	**G_c (kg/m^2s)**	**Liquid density (kg/m^3)**	**G_c (kg/m^2s)**
$\omega_{0.9}$ (JL) **PR EOS liquid density**	**619**	**6160**	**627**	**9780**	**812**	**46600**
Aspen ΔH (JG) **API liquid density (default)**	**600**	**5940**	**622**	**9700**	**767**	**45000**
Aspen vdP (JG) **API liquid density (default)**	**600**	**6090**	**624**	**9810**	**769**	**43970**

Case I - Cyclohexane

One-component

P_o = 10 bara (145 psia), T_o (saturation)

DIPPR (P-T, liquid density, latent heat, etc.)

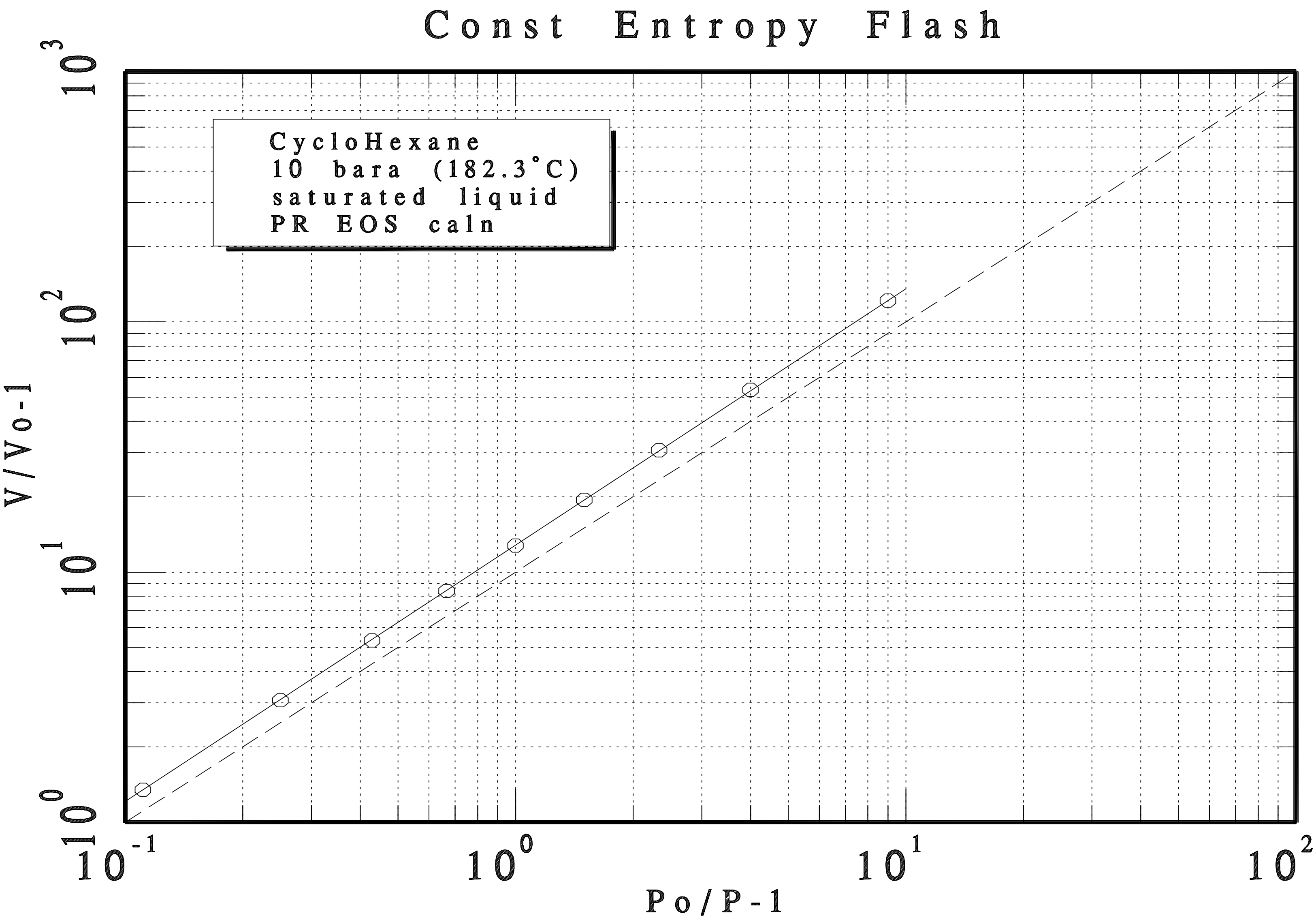
advantage: accurate P_{sat}, ρ_L, ΔH_{VL}
disadvantage: no data on H_L, H_V, S_L, S_V

EOS (SRK, PR) -

advantage: Z_L, Z_V, H_L, H_V, S_L, S_V
disadvantage: Z_L (5% off)

Case 1 – cyclo-C6 constant S flash

P BAR	T C	VL m3/kmol	VV m3/kmol	V/F mole quality	V 2ph m3/kmol
10	182.28	0.136	3.069	0.0	0.136
9	176.25	0.1337	3.424	0.0564	0.3193
8	169.69	0.1313	3.863	0.1131	0.5533
7	162.49	0.1289	4.422	0.1704	0.8603
6	154.46	0.1264	5.157	0.2289	1.2779
5	145.36	0.1239	6.171	0.2892	1.8727
4	134.76	0.1212	7.665	0.3524	2.7794
3	121.91	0.1183	10.102	0.4201	4.3121
2	105.21	0.1149	14.832	0.4955	7.4066
1	79.96	0.1107	28.372	0.5865	16.6852


Const Entropy Flash
CycloHexane
10 bara (182.3°C)
saturated liquid
PR EOS caln
V/Vo-1
Po/P-1
10^0
10^1
10^2
10^3
10^-1
10^0
10^1
10^2

Case I – Cyclo-C6 Preliminary Solution (Long Form)

PR EOS (P_c = 40.8 bar, T_c = 553.8K, acentric factor = 0.208)

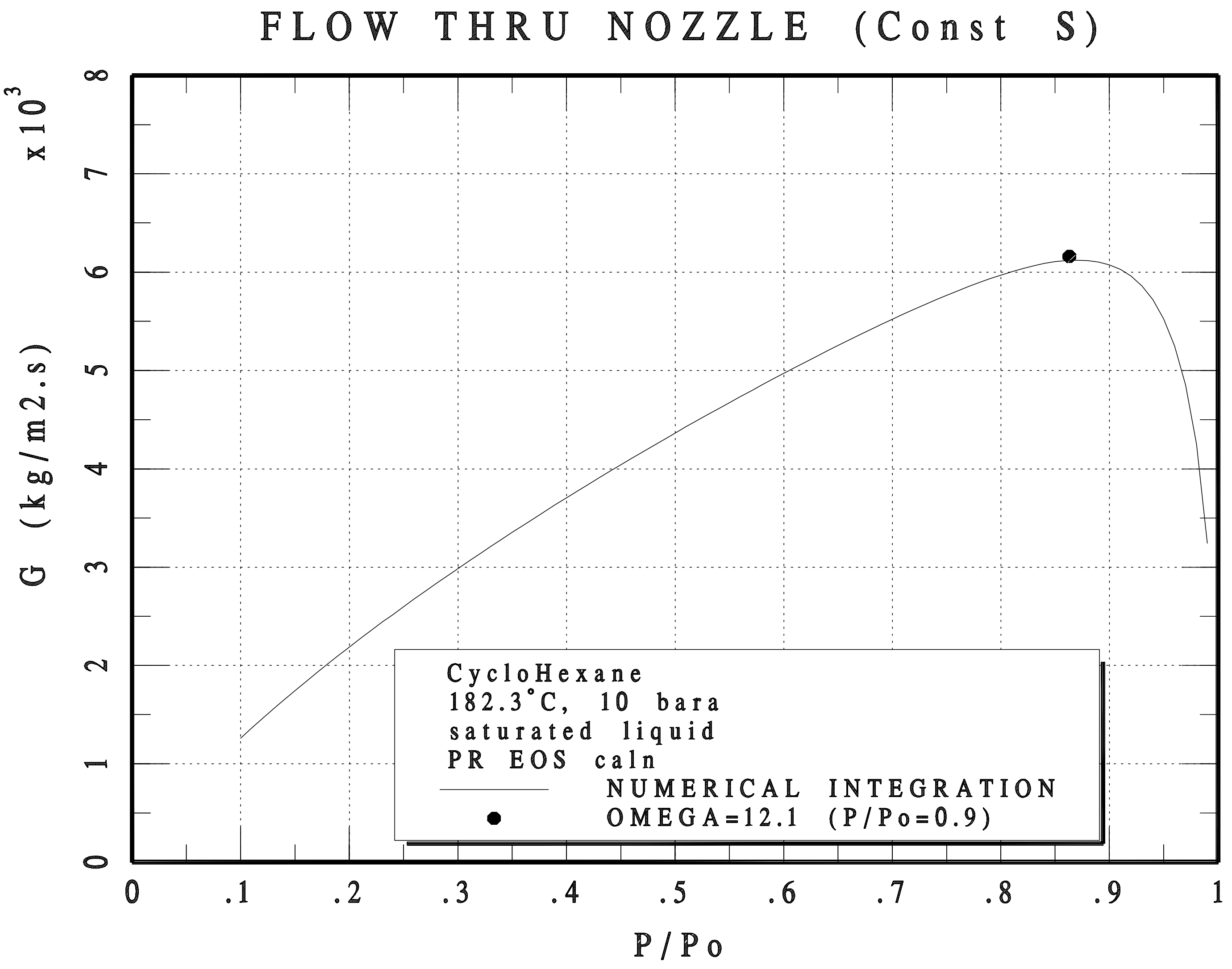
10 bar, 182.3°C, x_o = 0.0 (0.0001)

Constant S flash to 9 bar, 8 bar and so on

Curve fit P-v data

$$\left(\frac{v}{v_o}-1\right)=12.8\left(\frac{P_o}{P}-1\right)^{1.025}$$

Numerical integration of $\left[2\int_{P_o}^{P_t} -v\,dP\right]^{1/2} / v_t$ to seek max G


FLOW THRU NOZZLE (Const S)
G (kg/m2.s) x10^3
0
1
2
3
4
5
6
7
8
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
P/Po
CycloHexane
182.3°C, 10 bara
saturated liquid
PR EOS caln
NUMERICAL INTEGRATION
● OMEGA=12.1 (P/Po=0.9)

Case II – 20% mole Ethane / n-Heptane

Bubble-point prediction to match available literature VLE data on C2-C7 binary system -

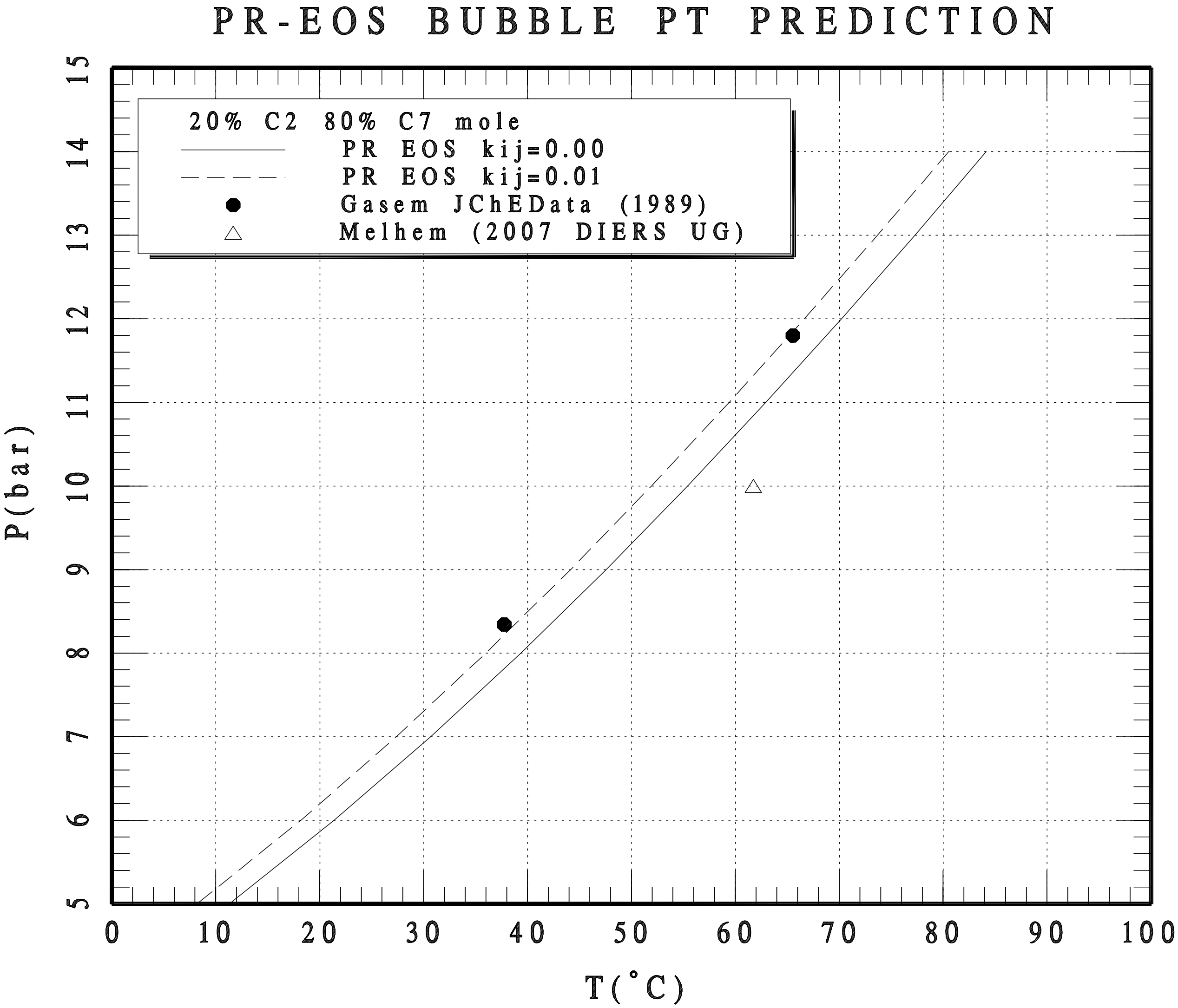
Kays, I&EC 30, 459 (1938)

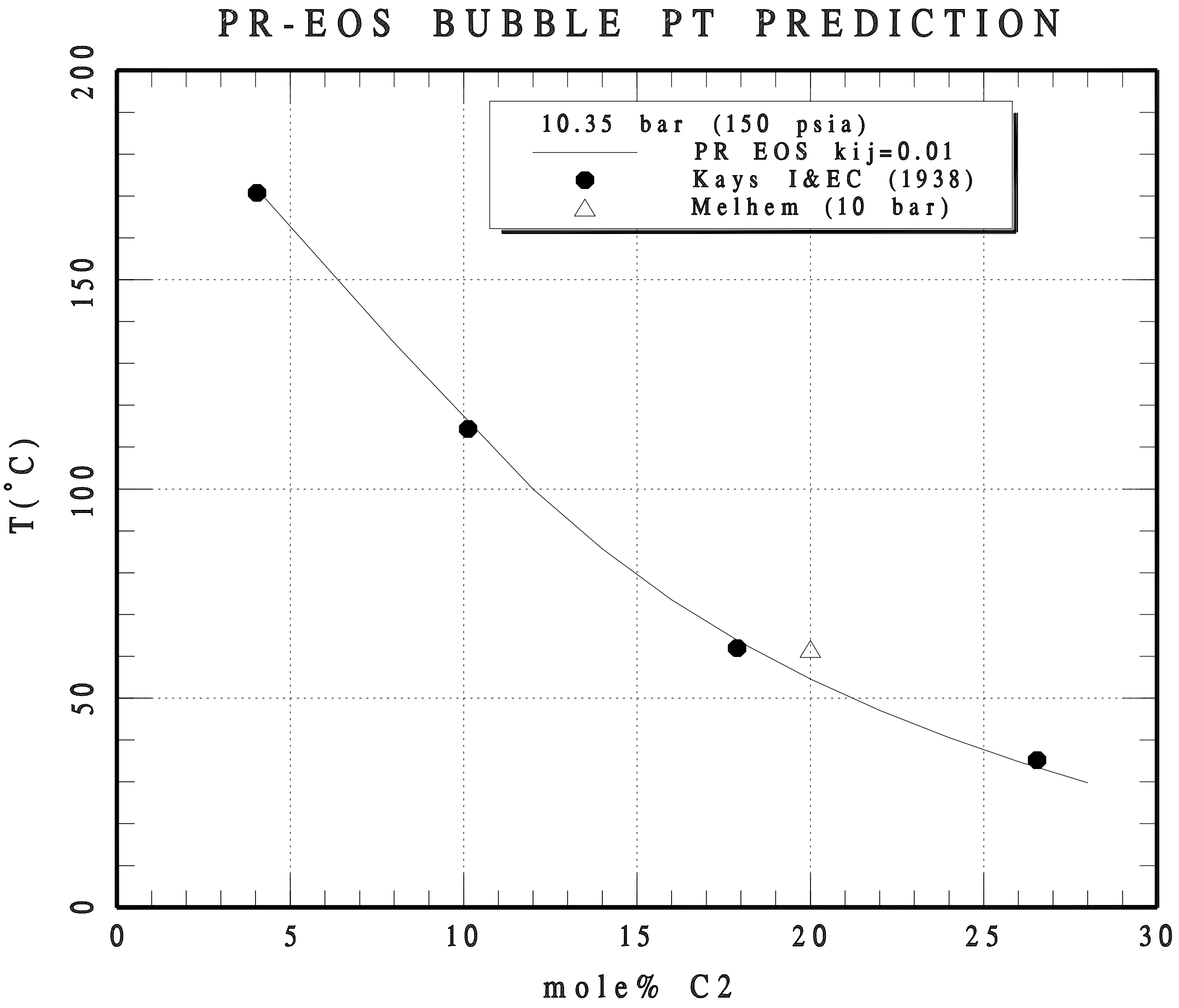
Gasem et. al., J Ch Eng Data, 34, 397 (1989)

PR EOS for C2-C7 binary

$k_{12} = 0.01$ (best fit)

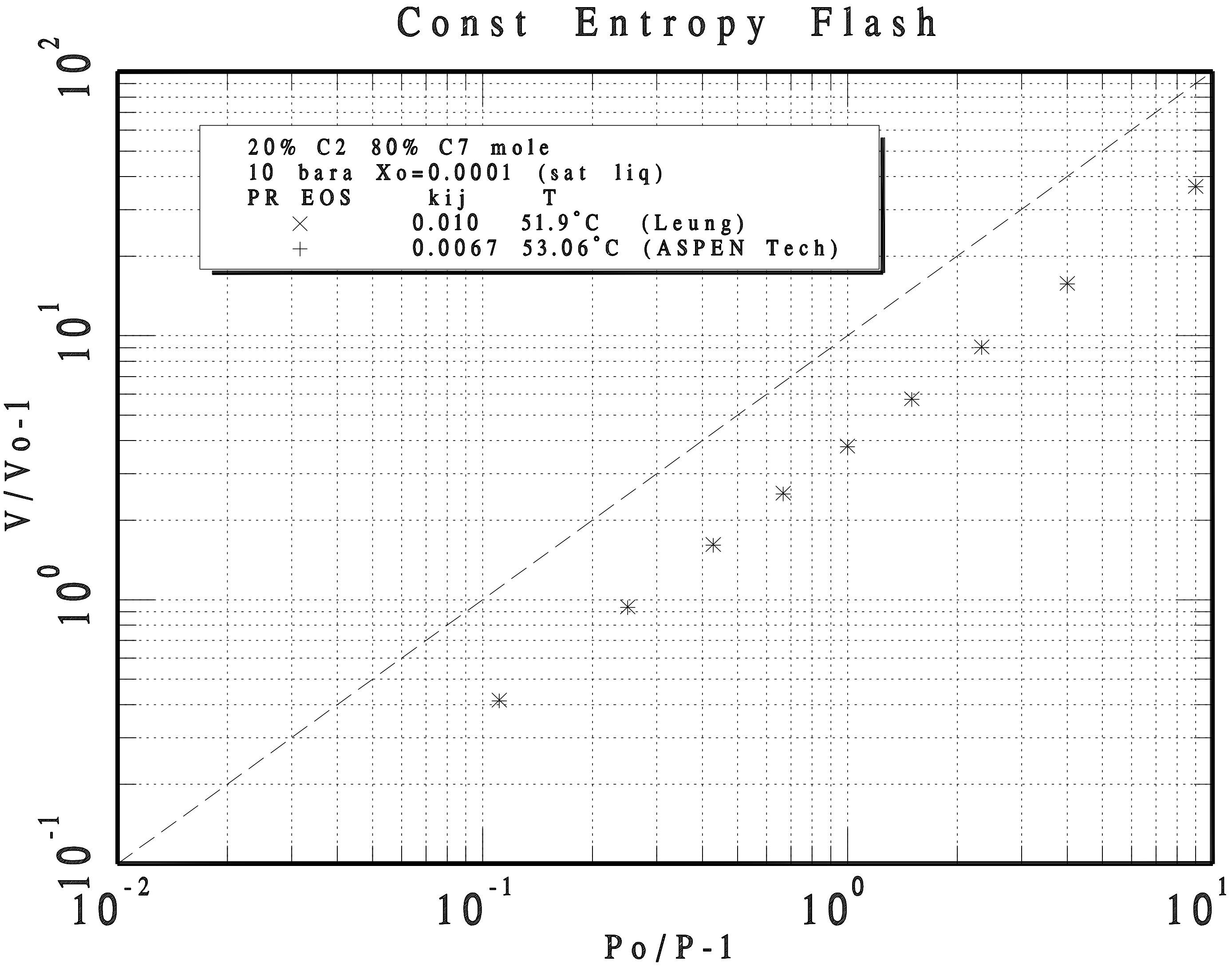
(caution - different value for SRK)


PR-EOS BUBBLE PT PREDICTION
20% C2 80% C7 mole
PR EOS kij=0.00
PR EOS kij=0.01
Gasem JChEData (1989)
Melhem (2007 DIERS UG)
P(bar)
T(°C)
5
6
7
8
9
10
11
12
13
14
15
0
10
20
30
40
50
60
70
80
90
100


PR-EOS BUBBLE PT PREDICTION
10.35 bar (150 psia)
PR EOS kij=0.01
Kays I&EC (1938)
Melhem (10 bar)
T(°C)
0
50
100
150
200
mole% C2
0
5
10
15
20
25
30

Case IIa – C2 / n-C7 constant S flash

P BAR	T C	X (C2) mole fr	Y (C2) mole fr	VL m3/kmol	VV m3/kmol	L/F mole liq/feed
10	51.92	0.2000	0.9752	0.13725	2.5025	0.99988
9	50.78	0.18317	0.97420	0.13837	2.7906	0.97872
8	49.58	0.16586	0.97284	0.13953	3.1245	0.96415
7	48.31	0.14794	0.97106	0.14074	3.6120	0.93676
6	46.94	0.12940	0.96865	0.14200	4.2264	0.91588
5	45.45	0.11012	0.96528	0.14330	5.0847	0.89490
4	43.75	0.09010	0.96031	0.14464	6.3683	0.87371
3	41.72	0.06922	0.95233	0.14600	8.4991	0.85191
2	39.02	0.04739	0.93754	0.14735	12.734	0.82856
1	34.35	0.02443	0.90041	0.14848	25.283	0.79958


Const Entropy Flash
20% C2 80% C7 mole
10 bara Xo=0.0001 (sat liq)
PR EOS kij T
× 0.010 51.9°C (Leung)
+ 0.0067 53.06°C (ASPEN Tech)
V/Vo-1
10^2
10^1
10^0
10^-1
10^-2
10^-1
10^0
10^1
Po/P-1

Case II C2-C7 Preliminary Solution (Long Form)

PR EOS (20% mole C2 in n-C7)

10 bara, 51.9°C, x_o = 0.0 (0.0001)

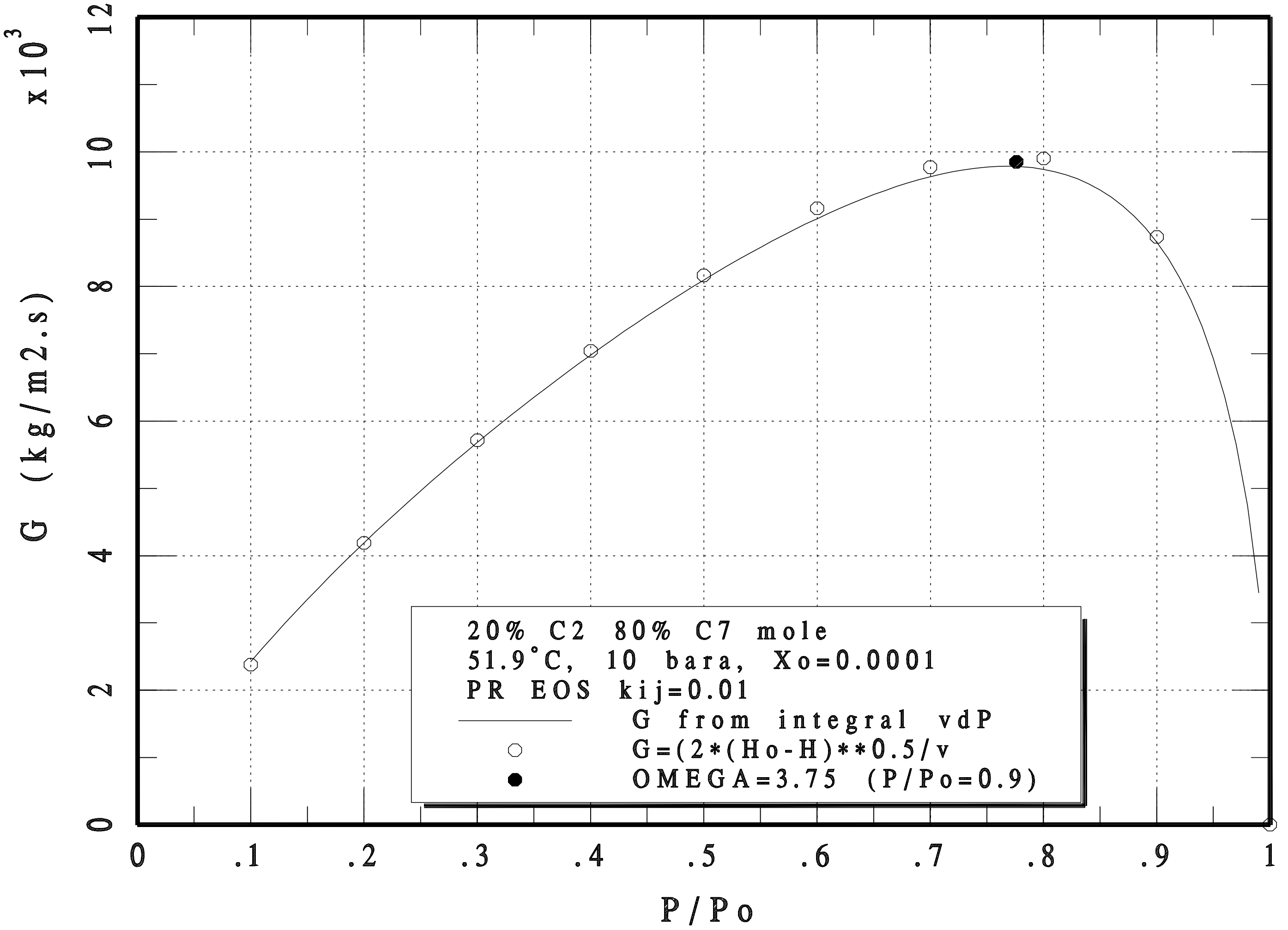
Constant S flash to lower pressures

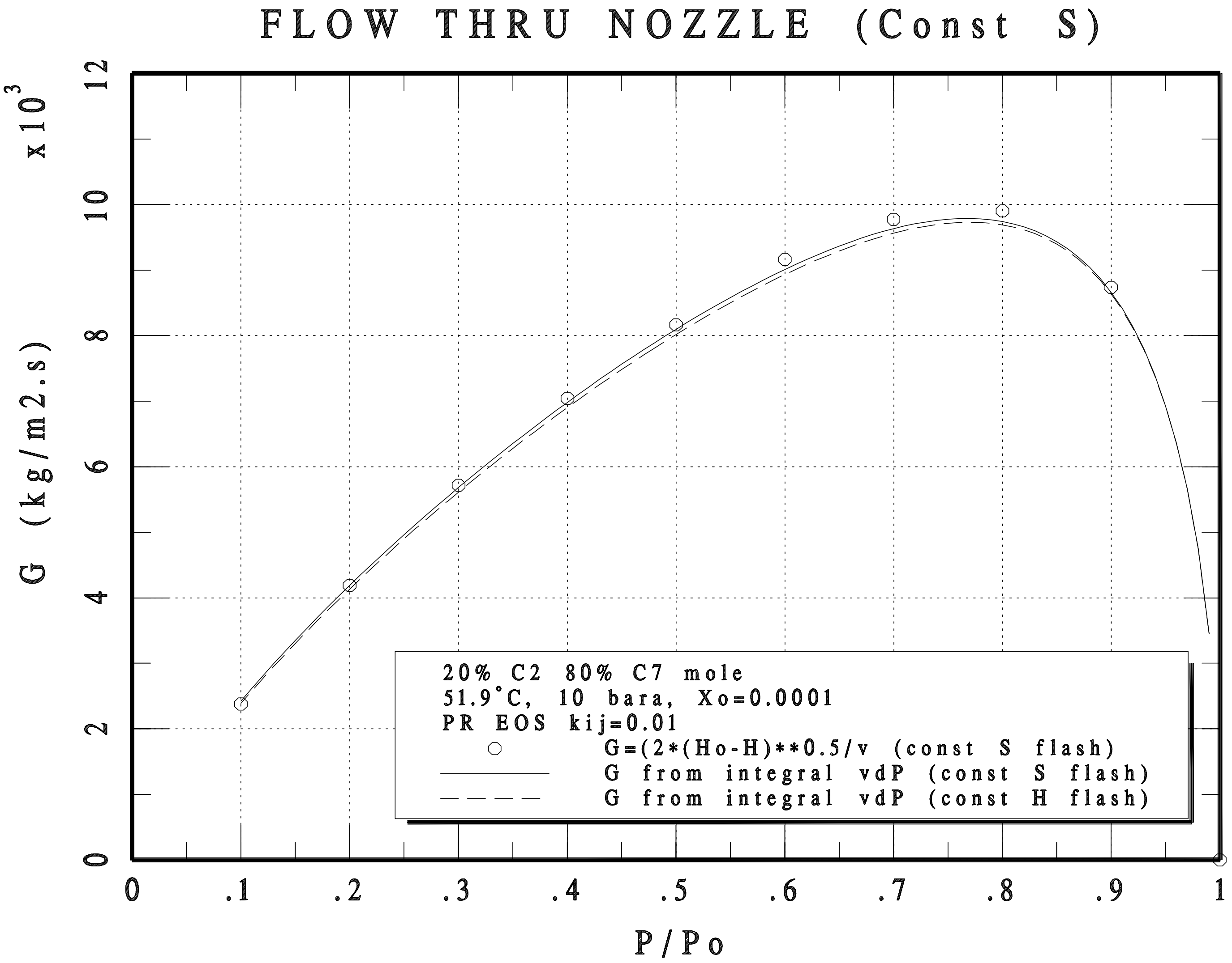
Curve fit P-v data

$$\left(\frac{v}{v_o}-1\right)=3.87\left(\frac{P_o}{P}-1\right)^{1.015}$$

Numerical integration of $\left[2\int_{P_o}^{P_t} - v\,dP\right]^{1/2} / v_t$ to seek max G

FLOW THRU NOZZLE (Const S)




FLOW THRU NOZZLE (Const S)
G (kg/m2.s)
x 10^3
0
2
4
6
8
10
12
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
P/Po
20% C2 80% C7 mole
51.9°C, 10 bara, Xo=0.0001
PR EOS kij=0.01
○ G=(2*(Ho-H)**0.5/v (const S flash)
G from integral vdP (const S flash)
G from integral vdP (const H flash)

Case III - N_2 / Cyclo-C6

Bubble-point prediction using PR EOS to match available N_2 solubility data in cyclo-C6 :

Hildebrand, JACS, 71, 3147 (1949)

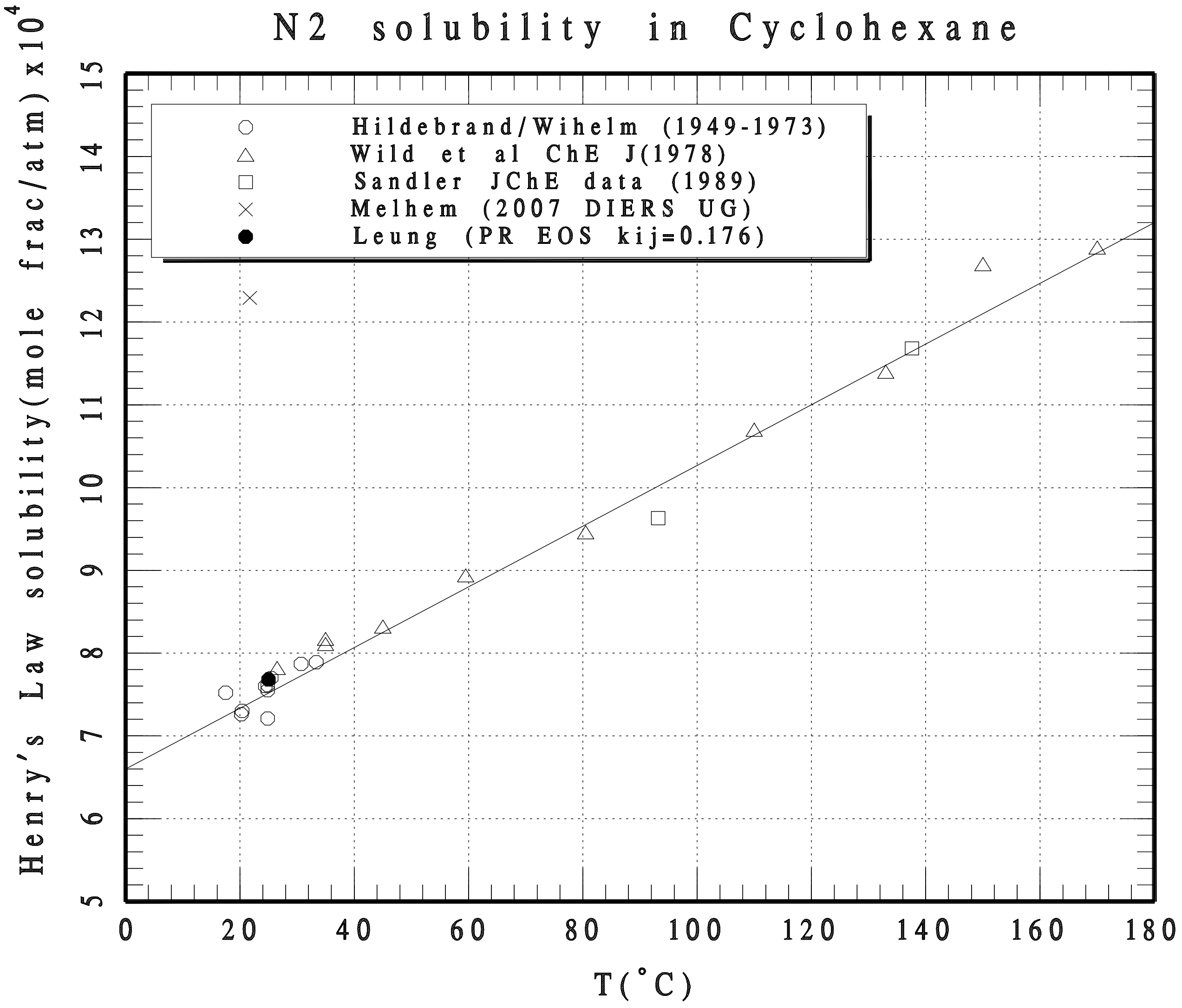
Hildebrand, I&EC Fund 6, 130 (1967)

Wilhelm, Chem Rev, 1, 73 (1973)

Wild, Ch E J, 15, 209 (1978)

Sandler, J Ch E Data, 34, 419 (1989)

Determine initial condition and k_{12} (BIP) for this mixture.


N2 solubility in Cyclohexane
○ Hildebrand/Wihelm (1949-1973)
△ Wild et al ChE J(1978)
□ Sandler JChE data (1989)
× Melhem (2007 DIERS UG)
● Leung (PR EOS kij=0.176)
Henry's Law solubility(mole frac/atm)x10^4
5
6
7
8
9
10
11
12
13
14
15
0
20
40
60
80
100
120
140
160
180
T(˚C)

PR EOS for N_2 / cyclo-C6 binary

$P_o = 33$ bar

$T_o = 25°C$

Henry's Law constant for N2 / cyclo-C6 pair -

7.68×10^{-4} mole frac/atm (solubility form: $x = H P$)

1320 bar/mole frac (volatility form: $P = H^* x$)

N_2 mole frac = 7.68×10^{-4} (33 x 0.9864 atm)

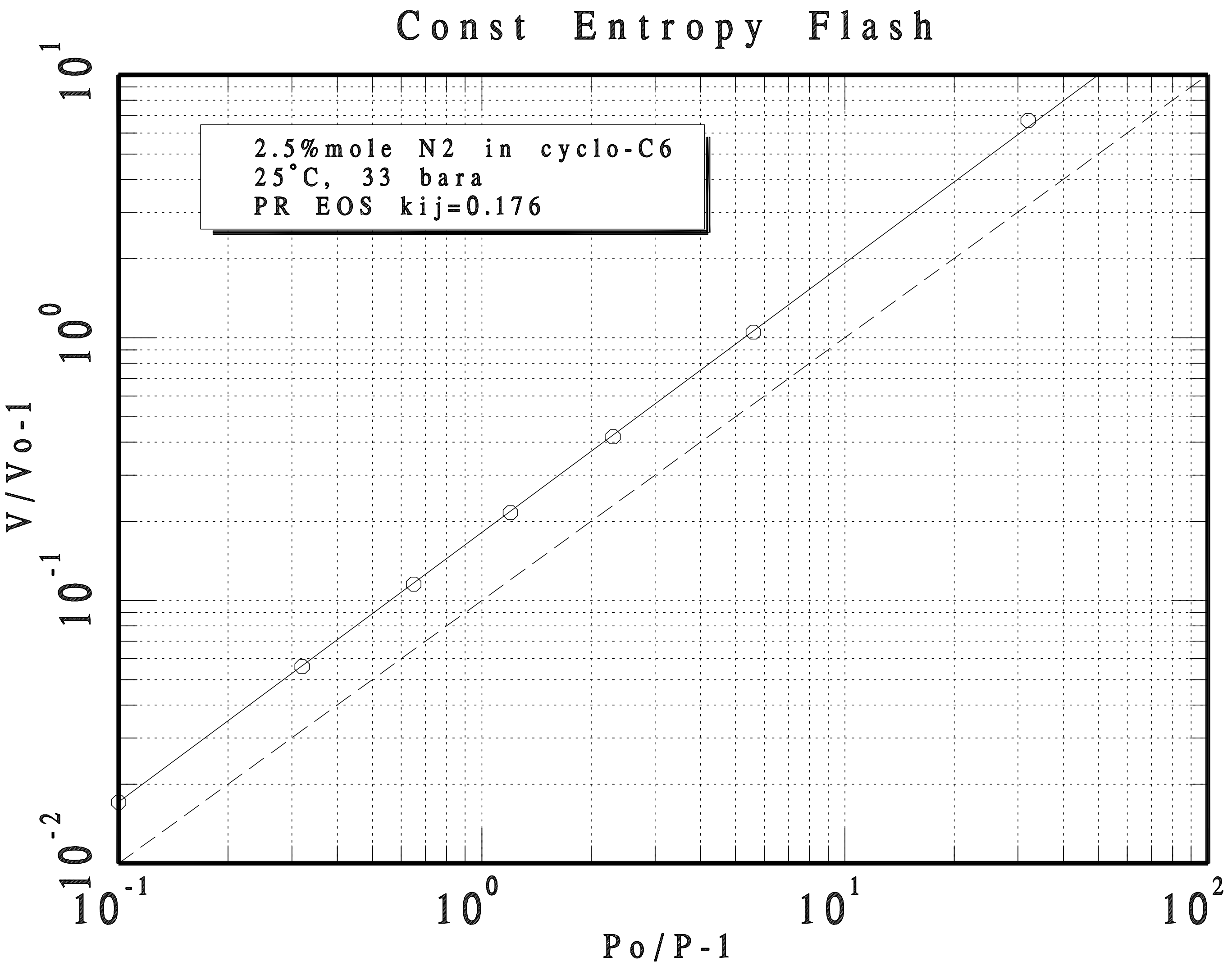
= 0.025, 2.5%

Best estimate $k_{12} = 0.176$ (PR EOS)

(caution - different value for SRK)

Case III – N2 cyclo-C6 const S flash

P bar	T C	X (N2) mole fr	Y (N2) mole fr	VL m3/kmol	VV m3/kmol	L/F mole liq/feed
33	25.00	0.025	0.9936	0.10187	0.74148	0.99999
30	24.96	0.0228	0.9932	0.1020	0.81612	0.99773
25	24.87	0.0191	0.9923	0.10228	0.98041	0.99395
20	24.76	0.0154	0.9911	0.10254	1.22696	0.99013
15	24.62	0.0116	0.9889	0.10279	1.6380	0.98627
10	24.41	0.00774	0.9845	0.10304	2.4599	0.98233
5	24.02	0.00384	0.9714	0.10328	4.9233	0.97813
1	22.6	6.92E-4	0.8727	0.10335	24.5323	0.97212


Const Entropy Flash
2.5%mole N2 in cyclo-C6
25°C, 33 bara
PR EOS kij=0.176
V/Vo-1
10^1
10^0
10^-1
10^-2
10^-1
10^0
10^1
10^2
Po/P-1

***Case III N2 / Cyclo-C6* Preliminary Solution (Long Form)**

PR EOS (2.5% mole N_2 in cyclo C6)

33 bara, 25°C, $x_o = 0.0$ (0.0001)

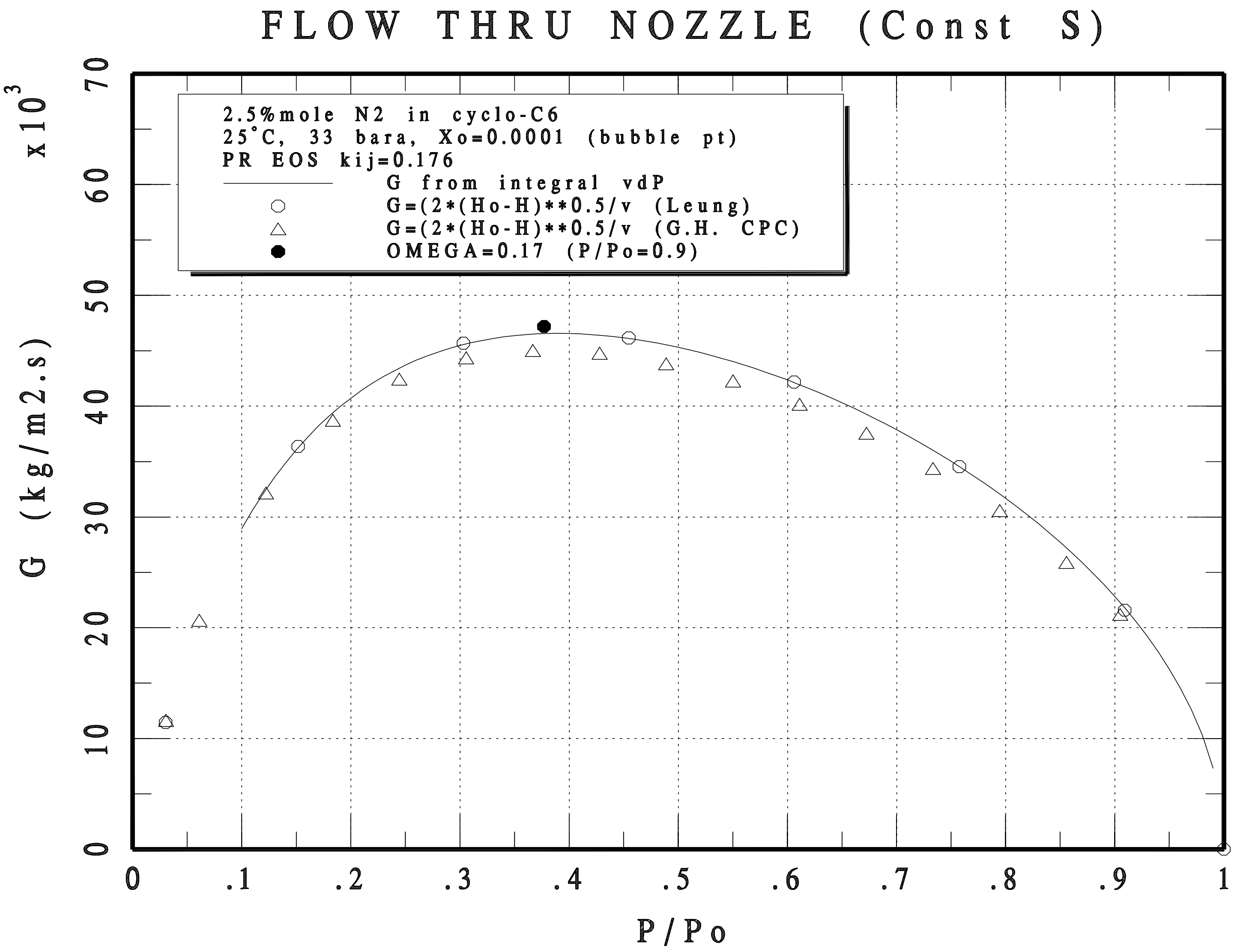
Constant S flash to lower pressures

Temperature stays relatively unchanged (expected)

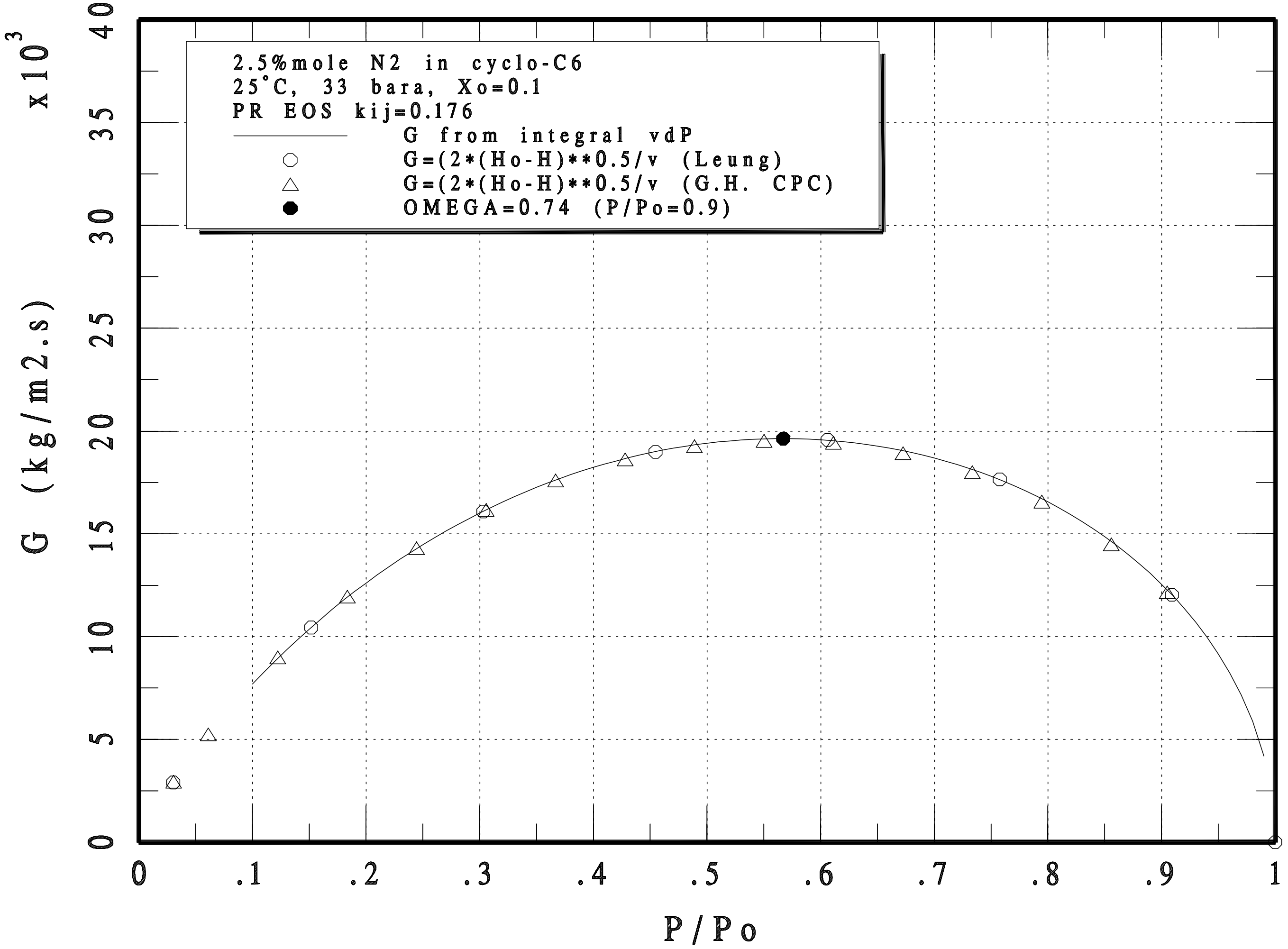
Curve fit P-v data

$$\left(\frac{v}{v_o} - 1\right) = 0.181\left(\frac{P_o}{P} - 1\right)^{1.025}$$

Numerical integration of $\left[2\int_{P_o}^{P_t} -v\,dP\right]^{1/2} / v_t$ to seek max G


FLOW THRU NOZZLE (Const S)
2.5%mole N2 in cyclo-C6
25°C, 33 bara, Xo=0.0001 (bubble pt)
PR EOS kij=0.176
G from integral vdP
G=(2*(Ho-H)**0.5/v (Leung)
G=(2*(Ho-H)**0.5/v (G.H. CPC)
OMEGA=0.17 (P/Po=0.9)
G (kg/m2.s)
x10^3
0
10
20
30
40
50
60
70
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1
P/Po

FLOW THRU NOZZLE (Const S)



100% c-C6, 10 bar, 182.3°C (selected data)

Method (initials)	**Case Ia $x_o = 0.0001$**		**Case Ib $x_o = 0.01$**		**Case Ic $x_o = 0.1$**	
	G_c (kg/m²s)	**η_c**	**G_c (kg/m²s)**	**η_c**	**G_c (kg/m²s)**	**η_c**
ω_o (JL - stagnation)	6140	0.863	6020	0.849	5190	0.778
$\omega_{0.9}$ (JL – 0.9)	6160	0.863	6020	0.849	5210	0.777
$\omega_{0.9}$ (DS – 0.9)	6090	0.862	5970	0.850	5190	0.779
vdP (JL - numerical)	6120	0.870	5990	0.857	5180	0.780
vdP (DS - numerical)	6070	0.870	5990	0.857	5170	0.790
vdP (DS - Simpson)	6070	0.865	5940	0.854	5170	0.784
Aspen ΔH (GH)	5940	0.845	5810	0.835	5100	0.794
VENT (NP)	6150	0.867	6010	0.853	5200	0.795
SIMSCI ΔH (WG)	6050	0.860	NA	NA	NA	NA
SUPERCHEM vdP (EK)	6060	0.875	5930	0.850	5140	0.775
vdP (HF)	5850	0.873	5720	0.862	4940	0.793
Mean Value	**6060**	**0.864**	**5940**	**0.852**	**5150**	**0.785**
Std. Dev.	**94**	**0.008**	**99**	**0.007**	**80**	**0.008**

20% C2/n-C7 (Liq. Comp.), 10 bar, 51.9°C (selected data)

Method (initials)	**Case IIa x_o = 0.0001**		**Case IIb x_o = 0.01**		**Case IIc x_o = 0.1**	
	G_c (kg/m^{2}s)	**η_c**	**G_c (kg/m^{2}s)**	**η_c**	**G_c (kg/m^{2}s)**	**η_c**
$\omega_{0.9}$ (JL)	9850	0.762	8940	0.733	5650	0.652
$\omega_{0.9}$ (DS)	9810	0.748	8930	0.722	5660	0.648
vdP (JL – numerical)	9780	0.768	8890	0.738	5650	0.650
vdP (DS – numerical)	9770	0.748	8890	0.730	5650	0.658
vdP (DS - Simpson)	9770	0.753	8890	0.727	5650	0.650
CHEMCAD (DS)	**8370**	0.709	8890	0.723	5660	0.649
ASPEN ΔH (GH)	9700	0.783	8800	0.731	5600	0.659
VENT (NP)	9180	0.750	8500	0.717	5670	0.640
SIMSCI ΔH (WG)	9870	0.755	NA	NA	NA	NA
SUPERCHEM vdP (EK)	9960	0.750	8980	0.725	5690	0.651
vdP (HG)	9840	0.756	8880	0.730	5510	0.656
Mean Value	**9630**	**0.753**	**8860**	**0.728**	**5640**	**0.651**
Std. Dev.	**463**	**0.018**	**135**	**0.006**	**51**	**0.006**

2.5% N_2/c-C6 (Liq. Comp.), 33 bar, 25°C (selected data)

Method (initials)	**Case IIIa x_o = 0.0001**		**Case IIIb x_o = 0.01**		**Case IIIc x_o = 0.1**	
	G_c (kg/m²s)	**η_c**	**G_c (kg/m²s)**	**η_c**	**G_c (kg/m²s)**	**η_c**
$\omega_{0.9}$ (JL)	47190	0.377	38050	0.456	19630	0.567
$\omega_{0.9}$ (DS)	46000	0.375	37440	0.452	20050	0.564
vdP (JL - numerical)	46600	0.390	37800	0.460	19630	0.566
vdP (DS - numerical)	45740	0.379	37330	0.457	20060	0.554
vdP (DS - Simpson)	45700	0.383	37320	0.455	20060	0.563
CHEMCAD(DS)	45750	0.382	37330	0.455	19960	0.566
ASPEN ΔH (GH)	45000	0.382	37000	0.458	19550	0.565
VENT (NP)	44800	0.355	40730	0.403	22040	0.494
SIMSCI ΔH (WG)	44990	0.385	NA	NA	NA	NA
SUPERCHEM (EK)	45850	0.379	37600	0.455	19570	0.561
Mean	**45760**	**0.379**	**37840**	**0.450**	**20060**	**0.556**
Std. Dev.	**740**	**0.009**	**1120**	**0.018**	**770**	**0.023**

Uncertainties in various models

- Case II bubble point calculation – 61.7°C (RD) vs 51.9°C(EK), perhaps due to different k_{ij} value, however G not much affected.
- NIST, DIPPR, PR-EOS would yield close agreement in P-T saturation, but not always in liquid density, however G not much affected.
- Chemcad uncertainty in its calculation method (DS will follow up).

FINDINGS

- Good agreement so far for all cases. Flash results are quite consistent.
- G based on ΔH from const S flash and integral vdP should yield consistent result, even for multicomponent system.
- Integral vdP method much more forgiving, even const H flash would yield close enough solution (not true approaching high quality flow).
- N_2-cHex case PR $k_{ij} = 0.176$ and NRTL model yield quite similar solutions.

Next DIERS UG Round-Robin

- Non-equilibrium (or frozen) nozzle flow ?
- Slip-equilibrium nozzle flow?
- Extend to pipe flow of various length ?
- Supercritical discharge?

Next Benchmark

- Pipe discharge mass flux calculations
- HEM (homogeneous-equilibrium model) assumption.
- Same 3 systems, 3 inlet qualities

  $x_o = 0.0001, 0.01, 0.1$
- 2 pipe configurations -

  $N = K_{en} + 4f_F\ L/D = 1.5 \quad (L/D = 50)$

  $N = K_{en} + 4f_F\ L/D = 5 \quad (L/D = 225)$

  fully turbulent two-phase, $f_F = 0.005$ (Fanning)

  sharp-edge entrance, $K_{en} = 0.5$