DIERS Users Group Discharge Flow Calculations – A Round-Robin Exercise

As part of the DIERS UG Design/Testing committee activity, a round-robin exercise is proposed in connection with discharge flow calculations for three fluid mixtures:

(I) cyclohexane (c-C6) at 10 bar abs (single component)

(II) 20% mole ethane in heptane (C2/n-C7) at 10 bar abs (two component)

(III) 2.5% mole nitrogen in cyclohexane (N2/c-C6) at 33 bar abs (two component)

For this exercise, a perfect-nozzle discharge is assumed with complete thermodynamic equilibrium and no slip between phases. Thus the classical homogeneous equilibrium model (HEM) should be followed. By fixing the flow regime, this allows us to check the variability of the calculations and the results. The proposed discharge flow inlet (stagnation) conditions are as follows:

Proposed inlet conditions

Case	Liquid Composition (mole)	P_o (bar)	T_o (°C)	x_o (vapor mass frac.)
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

- Note that only the liquid composition is given and is held constant for each case with varying vapor mass fraction x_o.

- For Case I the initial pressure P_o and temperature T_o (10 bar abs, 182.3ºC) fall on the saturation line for c-C6 for a single-component system.

- For Case II, the $P_o - T_o$ pair (10 bar abs, 51.9ºC) has been chosen to match available bubble points for a 20% C2/80% n-C7 mixture, see papers by Kays (1938) and Gasem (1989), and attached Figures 1 and 2. If the Peng-Robinson (PR) EOS is used, the best-fit binary-interaction coefficient k_{ij} is 0.01. Note that a different k_{ij} value would be needed for other EOS such as Soave-Redlich-Kwong (SRK).

- For Case III, the $P_o - T_o$ pair (33 bar abs, 25ºC) has been chosen to match available N_2 solubility data in c-C6. Figure 3 shows the Henry's law solubility data from literature. At 25ºC, the solubility form x = HP gave a Henry's law constant of 7.68 x 10^{-4} mole frac/atm. Thus at a pressure of 33 bar (32.55 atm), the N_2 mole fraction is x = HP = 0.025 or 2.5%. Using the PR EOS, the best fit k_{ij} is 0.176 for this condition. Again a different k_{ij} value would be expected using the SRK EOS.

Data Submission should include a summary sheet listing methods or calculational steps, vapor-liquid equilibrium model used in Cases II and III, flash calculations (an example is shown in Table 1), and most important of all the discharge mass flux G (kg/m^2s) and choking pressure (bar abs) for all nine inlet conditions.

Data please Email to Joseph Leung at leunginc@cox.net

NO LATER THAN OCT 1st 2008

Some preliminary results have been obtained but the deadline is extended to have more participation. Results will be presented at the next DIERS Users Group meeting in San Antonio, Oct 20-22,2008.

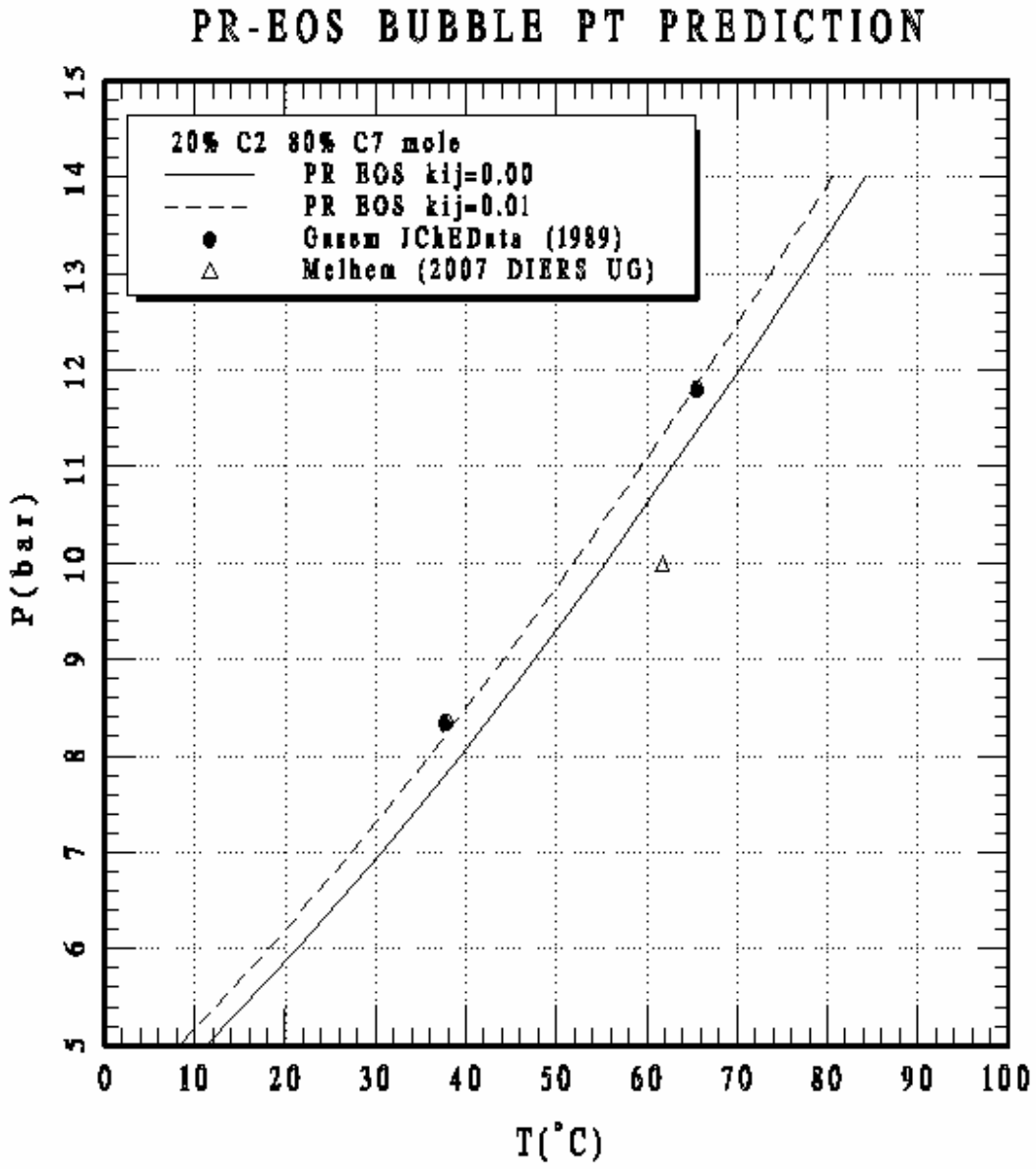

Figure 1 Bubble point data for 20% ethane in n-heptane from Gasem (1989) showing PR EOS prediction with two different k_{ij} values (0 and 0.01).
Ref.: K. A. M. Gasem et al., J. Chem. Eng. Data 34, 397-398 (1989).

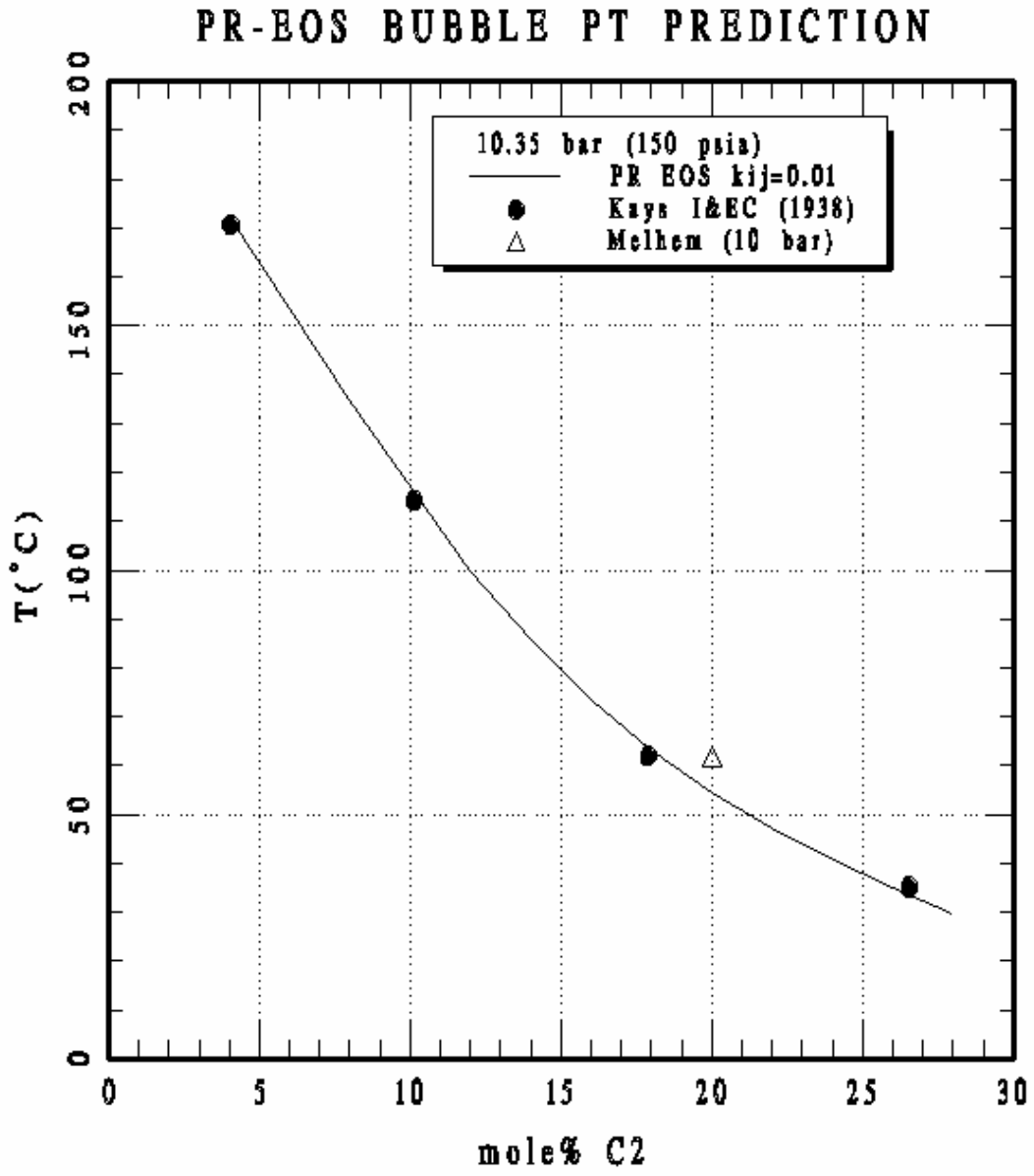

Figure 2 Bubble point temperature versus ethane mole percent data of Kays (1938) at 10.33 bar – also showing PR EOS prediction with $k_{ij} = 0.01$ for the ethane-heptane binary mixture. *Ref.: W. B. Kay, Ind Eng. Chem 30, 459-465 (1938).*

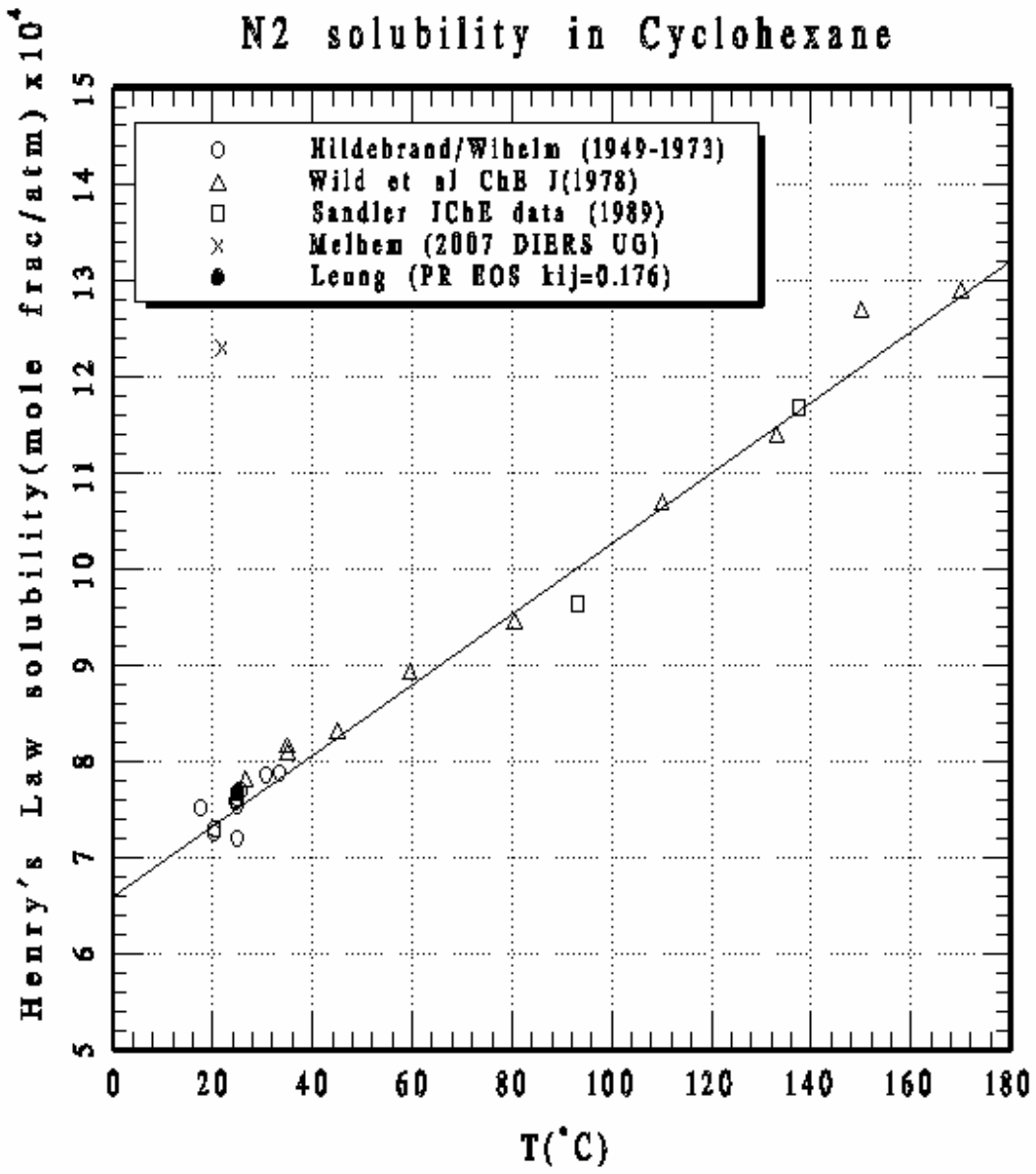

Figure 3 N_2 solubility data in cyclohexane.

Ref.: *J. Wild et al., Chem. Eng. J. 15, 209-214 (1978)*
J. D. Dymond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. 6, 130 (1967)
J. C. Gjaldbaek and J. H. Hildebrand, J. Am. Chem. Soc. 71, 3147 (1949)
E. Wilhelm and R. Battino, Chem. Rev. 1, 73 (1973)
S. K. Shibata and S. I. Sandler, J. Chem. Eng. Data 34, 419-424 (1989)

Table 1

A Sample of Constant Entropy Flash for Case IIa Showing at Decreasing Pressure the Corresponding Temperature, C2 Mole Fraction in Liquid and in Vapor, Liquid Molar Specific Volume, Vapor Molar Specific Volume and Liquid-to-Total L/F Mole Ratio

Case IIa – C2 / n-C7 constant S flash

P	T	X (C2)	Y (C2)	VL	VV	L/F mole
BAR	C	mole fr	mole fr	m3/kmol	m3/kmol	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