

Rovnováha v trojsložkové soustavě voda - benzén - kys. octová

Potřebná data: G_f^0 čistých složek
konstanty závislosti $G^E(x)$ ve všech binárních

Výsledek: predikce fázové rovnováhy

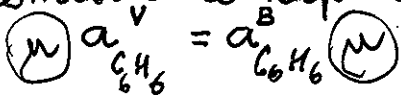
Porovnání s experimentem \rightarrow konstanty závislosti $G^E(x)$ v
termárním portoku.

Data: G_f^0 čistých složek - ma.ji.: Atkins: Phys. Chem. 4. vyd. 1990, s. 939, 943.
: Int. Crit. Tables, 1928
: Stull D.R., Westrum E.F., Sinke G.C.: The chem. thermod. (1972)
 $H_2O: -237.13 \text{ kJ} \cdot \text{mol}^{-1}$
 $C_6H_6: +124.30 \text{ kJ} \cdot \text{mol}^{-1}$
 $CH_3COOH: -389.90 \text{ kJ} \cdot \text{mol}^{-1}$
(nemí třeba přepočítat G_f^0 na jinou T.)

Závislost $G^E(x)$ - tabulky: Landolt, Bernstein 6. vyd. 1961, Bd. II/2a,
International Critical Tables, Vol. 3, s. 287

System benzén - voda: nemísitelné kapaliny

$$\mu_i = \mu_i^0 + RT \ln a_i$$



$$y_B^V x_B^V = x_B^B x_B^B$$

$$\downarrow \qquad \downarrow$$

$$0,00038 \qquad 0,9979$$

Stand. stav: $C_6H_6(l)$

$$G^E = A x_A x_B$$

$$\ln y_B^V = A \frac{(x_B^V)^2}{(1-x_B^V)^2}$$

$$-\ln y_B^B = A \frac{(x_B^B)^2}{(1-x_B^B)^2}$$

Dosažením:

$$A(1-x_B^V)^2 + \ln x_B^V = A(1-x_B^B)^2 + \ln x_B^B$$

$$A = \frac{\ln(x_B^B/x_B^V)}{[(1-x_B^V)^2 - (1-x_B^B)^2]} = 7,879$$

$$G^E = 7,879 \cdot RT \cdot x_B \cdot x_V = 19194 \cdot x_B \cdot x_V \quad (T=298K)$$

System voda - kys. octová:

P_{H_2O}/torr	$x_{H_2O}^l$	$a_{H_2O}^l = \frac{P_{H_2O}^l}{P_{H_2O}^0}$	γ_{H_2O}
0	0	0	\sim
16,4	0,146	0,267	1,832
35,2	0,431	0,574	1,333
44,2	0,691	0,721	1,125
51,4	0,772	0,838	1,086
58,3	0,937	0,951	1,015
61,3	1,000	1	1

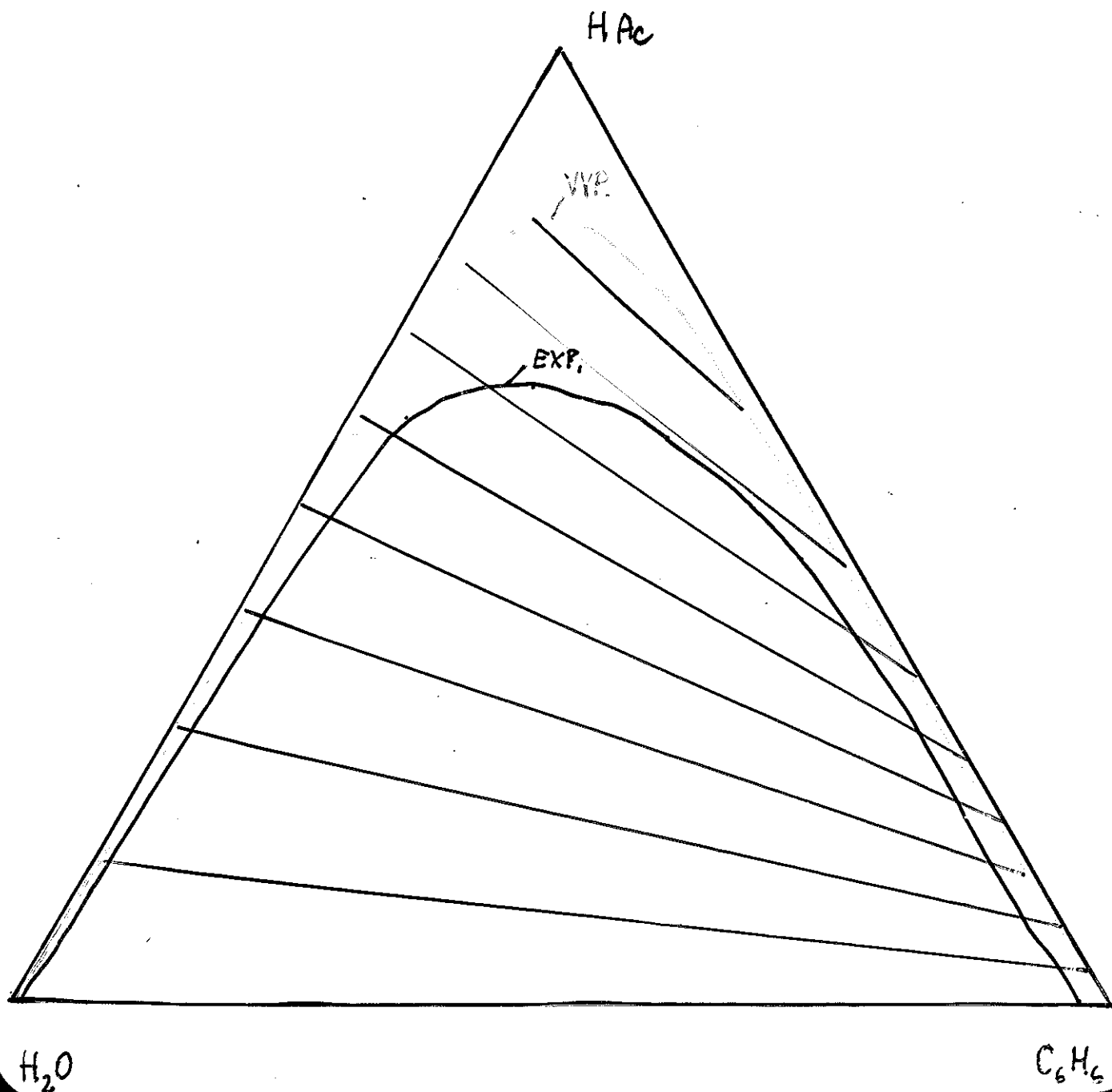
(oligomerace zanedbána)

Interaction parameters of high order:
A₂, B₂, A₃
0.0 0.0 0.0

naležt porovnáním s exp.

2. Fáze v rovnováze = identicky LIQUID!

výsledek: ter. diagram - predikce.



DATE 11/ 7/1995

SYSTEM: AQ-BE-AC-
EQUILIBRIUM: Liquid Liquid
Number of TIE-angles: 1
TIME 16:10: 8.82

>>computed values<<

wabc potadi

1 TIE-angle:
T= 299.15[K] G syst.= -188390.9688761562000[J] MAX INT. NFV= 400
global cont. [%] Liquid Liquid
AQ 10.0000 .14647287/ 29.26374653
BE 45.0000 67.24531259 1.51018590
AC 45.0000 32.60821454 69.22606757
phase ratio []: .49685029 .50314971
phase en. [J]: -.765746E+05 -.298807E+06
TIME 16:10: 9.21

computed by PD_* (3.14) using: ac_aq_be.fdc
(ac_aq_be.pdd)
(ac_aq_be.par)

DATE 11/ 7/1995

SYSTEM: AC-AQ-BE-
EQUILIBRIUM: Liquid Liquid
Number of TIE-angles: 1
TIME 16:15:30.36

>>computed values<<

ABC potadi

1 TIE-angle:
T= 299.15[K] G syst.= -188390.9688736053000[J] MAX INT. NFV= 165
global cont. [%] Liquid Liquid
AC 45.0000 69.22406944 32.61075919
AQ 10.0000 29.26603338 .14651409/
BE 45.0000 1.50989717 67.24272672
phase ratio []: .50312499 .49687501
phase en. [J]: -.298804E+06 -.765890E+05
TIME 16:15:30.63

computed by PD_* (3.14) using: ac_aq_be.fdc
(ac_aq_be.pdd)
(ac_aq_be.par)

DATE 11/ 7/1995

SYSTEM: AC-AQ-BE-
EQUILIBRIUM: Liquid Liquid
Number of TIE-angles: 1
TIME 16:17:45.53

Base: AQ

>>computed values<<

1 TIE-angle:
T= 299.15[K] G syst.= -188390.9688752844000[J] MAX INT. NFV= 270
global cont. [%] Liquid Liquid
AC 45.0000 69.22780750 32.60597639
AQ 10.0000 29.26172405 .14643555/
BE 45.0000 1.51046845 67.24758807
phase ratio []: .50317158 .49682842
phase en. [J]: -.298810E+06 -.765619E+05
TIME 16:17:45.86

computed by PD_* (3.14) using: ac_aq_be.fdc
(ac_aq_be.pdd)
(ac_aq_be.par)

PARAMETERS OF THE VODA-BENZEN-OCTOVA SYSTEM

POČITA' ✓

Source: LANDOLT-BERNSTEIN TAB.

*****PHASE:LIQUID4 *****

Model: Number of sublatices: 1
 Number of components: 3
 sublattice Stoich.koef. Schematic view
 1 1.0 AQ BE AC

THERMODYNAMIC PARAMETERS:

Reference level parameters:

AQ (298.15- 398.00K)
 1 -20840.685 0. 0. 0. 0. 0. 0. 0.
 BE (298.15- 398.00K)
 1 -51669.395 0. 0. 0. 0. 0. 0. 0.
 AC (298.15- 398.00K)
 1 -47644.37 0. 0. 0. 0. 0. 0. 0.

Interaction parameters of first order: included(Y/N) [Y]
 L0: L1: L2:

AQ,BE 19194.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 AQ,AC 2059.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 BE,AC 2315.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

\$ Interaction parameters of high order: included(Y/N) [N]
 AQ,BE,AC 0.0 0.0 0.0

\$ MAGNETIC PARAMETERS: included(Y/N) [N]

*****PHASE:LIQUID2 *****

Model: Number of sublatices: 1
 Number of components: 3
 sublattice Stoich.koef. Schematic view
 1 1.0 AQ BE AC

THERMODYNAMIC PARAMETERS:

Reference level parameters:

AQ (298.15- 398.00K)
 1 -20840.685 0. 0. 0. 0. 0. 0. 0.
 BE (298.15- 398.00K)
 1 -51669.395 0. 0. 0. 0. 0. 0. 0.
 AC (298.15- 398.00K)
 1 -47644.37 0. 0. 0. 0. 0. 0. 0.

Interaction parameters of first order: included(Y/N) [Y]
 L0: L1: L2:

AQ,BE 19000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 AQ,AC 2400.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 BE,AC 1900.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

\$ Interaction parameters of high order: included(Y/N) [N]
 AQ,BE,AC 0.0 0.0 0.0

\$ MAGNETIC PARAMETERS: included(Y/N) [N]

***** end ***** of file AQBEAC.par

VOBEOC.PAR 7 A-dis

SYSTEM: AQ-BE-AC-
 EQUILIBRIUM: LIQUID1 LIQUID2
 Number of TIE-angles: 11
 TIME 18: 5:48.66

>>computed values<<

1 TIE-angle:

T= 298.15[K] G syst.= -26669.9430054070800[J] MAX INT. NFV= 239
 global cont. [%] LIQUID1 LIQUID2
 AQ 49.9000 96.53210046 .18217722
 BE 50.0000 3.30953657 99.78004772
 AC .1000 .15836297 .03777505
 phase ratio []: .81717424 .18282576
 phase en. [J]: -.211249E+05 -.514548E+05
 TIME 18: 5:56.30

2 TIE-angle:

T= 298.15[K] G syst.= -28226.5422266501300[J] MAX INT. NFV= 123
 global cont. [%] LIQUID1 LIQUID2
 AQ 45.0000 81.48088420 .22870290
 BE 45.0000 3.65497701 95.74082903
 AC 10.0000 14.86413879 4.03046807
 phase ratio []: .81903752 .18096248
 phase en. [J]: -.230428E+05 -.516882E+05
 TIME 18: 6: 1.90

3 TIE-angle:

T= 298.00[K] G syst.= -29785.3588520370100[J] STEP TOL NFV= 181
 global cont. [%] LIQUID1 LIQUID2
 AQ 40.0000 67.89642456 .29516423
 BE 40.0000 4.13317701 91.04906235
 AC 20.0000 27.97039844 8.65577342
 phase ratio []: .82140511 .17859489
 phase en. [J]: -.250136E+05 -.517319E+05
 TIME 18: 6: 6.90

4 TIE-angle:

T= 298.00[K] G syst.= -31432.3198308309400[J] STEP TOL NFV= 139
 global cont. [%] LIQUID1 LIQUID2
 AQ 35.0000 55.64486180 .39530878
 BE 35.0000 4.82676344 85.57604863
 AC 30.0000 39.52837476 14.02864259
 phase ratio []: .82526639 .17473361
 phase en. [J]: -.271514E+05 -.516513E+05
 TIME 18: 6:10.30

5 TIE-angle:

T= 298.00[K] G syst.= -33207.8991301589300[J] MAX INT. NFV= 166
 global cont. [%] LIQUID1 LIQUID2
 AQ 30.0000 44.49160780 .55347440
 BE 30.0000 5.84736938 79.07744301
 AC 40.0000 49.66102282 20.36908259
 phase ratio []: .83204829 .16795171
 phase en. [J]: -.295302E+05 -.514274E+05
 TIME 18: 6:14.48

6 TIE-angle:

T= 298.00[K] G syst.= -35147.3155695423200[J] MAX INT. NFV= 139
 global cont. [%] LIQUID1 LIQUID2
 AQ 25.0000 34.20115193 .82376294
 BE 25.0000 7.43436012 71.15412038
 AC 50.0000 58.36448795 28.02211668
 phase ratio []: .84550536 .15449464
 phase en. [J]: -.322513E+05 -.509965E+05
 TIME 18: 6:18.65