

39. ZADATAK

Za sustav benzen (1) – *i*-propanol (2) određeni su parametri ravnotežnog stanja pri temperaturi od 25 °C:

x_1	0,076	0,164	0,300	0,479	0,638	0,854	0,941
y_1	0,365	0,530	0,635	0,712	0,745	0,765	0,877
p/mmHg	66,4	84,0	99,8	105,8	108,4	109,0	104,5

Ravnotežni tlakovi para čistih komponenata izračunavaju se Antoineovim izrazom:

$$\log_{10}(p^{\bullet}/\text{mmHg}) = A - \frac{B}{(T/^{\circ}\text{C}) + C},$$

uz parametre:

	A	B	C
benzen (1)	6,90565	1211,033	220,790
<i>i</i> -propanol (2)	7,75634	1366,142	197,970

Izračunati koeficijente aktiviteta obje komponenata za otopinu sastava $x_1=0,479$ (standardno stanje – čista tvar), uz pretpostavku da se otopina u pari vlada idealno, a u kapljevini prema van Laarovu modelu. Konstante van Laarova modela izračunati na temelju parametara azeotropne točke. Parametre azeotropne točke odrediti na temelju grafičkih prikaza funkcija $y_1=f(x_1)$ i $p=f(x_1, y_1)$.

RJEŠENJE

$\gamma=?$

benzen (1) – *i*-propanol (2)

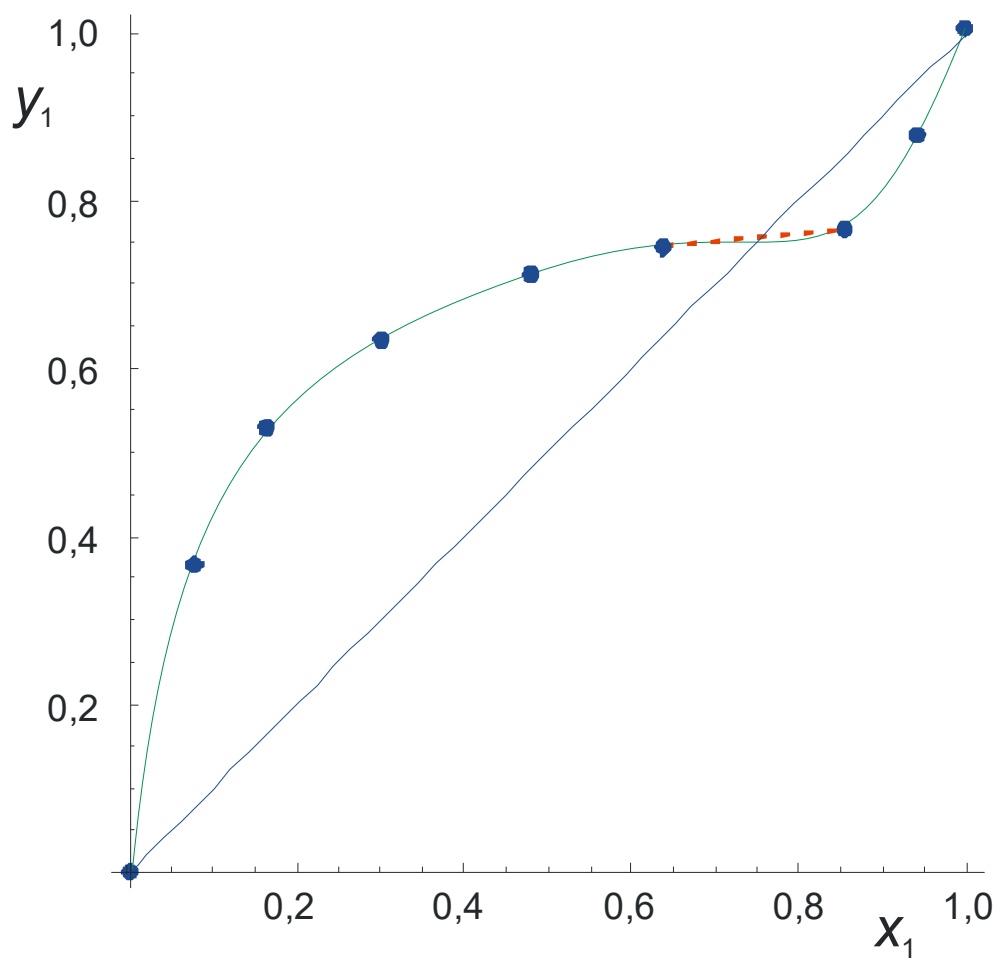
Azeotropna točka, Van Laar

Ravnotežni tlakovi čistih komponenata:

$$p_1^\bullet = 10^{A_1 - \frac{B_1}{(T/^\circ\text{C}) + C_1}} = 10^{6,90565 - \frac{1211,033}{25 + 220,790}} = 95,18 \text{ mmHg}$$

$$p_2^\bullet = 10^{A_2 - \frac{B_2}{(T/^\circ\text{C}) + C_2}} = 10^{7,75634 - \frac{1366,142}{25 + 197,970}} = 42,5911 \text{ mmHg}$$

xy-dijagram

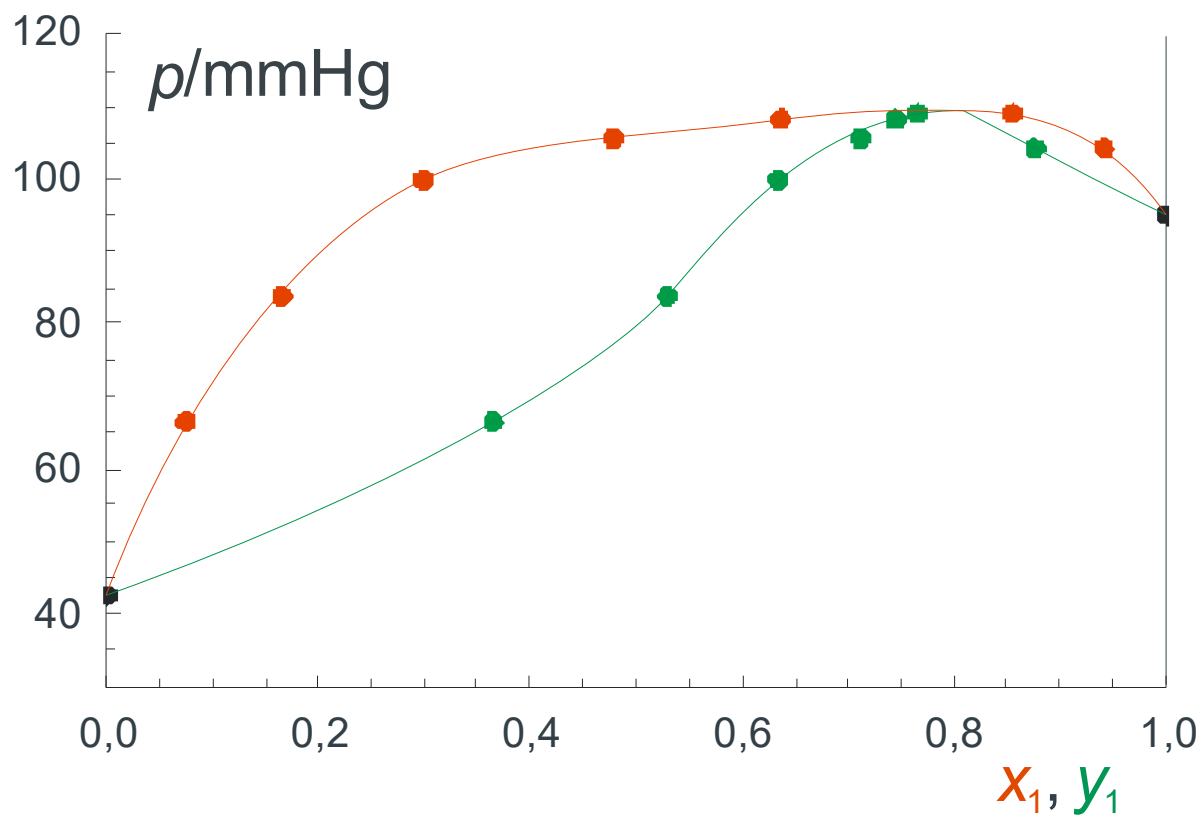


Linearnom interpolacijom:

$$x_{1,\text{az}} = 0,638 + \frac{0,854 - 0,638}{0,765 - 0,745} (y_{1,\text{az}} - 0,745)$$

$$x_{1,\text{az}} = y_{1,\text{az}} = 0,755918$$

Dijagram vrenja:



$$p_{az} \approx \max p = 109,0 \text{ mmHg}$$

Koeficijenti aktiviteta u azeotropnoj točki!

$$\frac{y_i}{x_i} = \frac{\gamma_i^L p_i^\bullet}{p} \exp\left[\frac{v_i^L(p - p_i^\bullet)}{RT}\right] \approx \frac{\gamma_i^L p_i^\bullet}{p}$$

$$py_i = x_i \gamma_i^L p_i^\bullet$$

$$\gamma_{1,az} = \frac{y_{1,az} p_{az}}{x_{1,az} p_1^\bullet} = \frac{p_{az}}{p_1^\bullet} = \frac{109,0}{95,18} = 1,1452$$

$$\gamma_{2,az} = \frac{y_{2,az} p_{az}}{x_{2,az} p_2^\bullet} = \frac{p_{az}}{p_2^\bullet} = \frac{109,0}{42,5911} = 2,55922$$

Parametri Van Laarova modela

$$A' = \ln \gamma_{1,\text{az}} \left[1 + \frac{(1 - x_{1,\text{az}}) \ln \gamma_{2,\text{az}}}{x_{1,\text{az}} \ln \gamma_{1,\text{az}}} \right]^2$$

$$A' = 1,1452 \left[1 + \frac{(1 - 0,755918) 2,55922}{0,755918 \cdot 1,1452} \right]^2 = 1,42149$$

$$B' = \ln \gamma_{2,\text{az}} \left[1 + \frac{x_{1,\text{az}} \ln \gamma_{1,\text{az}}}{(1 - x_{1,\text{az}}) \ln \gamma_{2,\text{az}}} \right]^2$$

$$B' = \ln 2,55922 \left[1 + \frac{0,755918 \ln 1,1452}{(1 - 0,755918) \ln 2,55922} \right]^2 = 1,96709$$

Koeficijenti aktiviteta preko Van Laarova modela

$$\ln \gamma_1 = \frac{A'}{\left(1 + \frac{A'x_1}{B'x_2}\right)^2},$$

$$\gamma_1 = \exp \left\{ \frac{1,42149}{\left[1 + \frac{1,42149 \cdot 0,479}{1,96709 \cdot (1 - 0,479)}\right]^2} \right\} = 1,67053$$

$$\ln \gamma_2 = \frac{B'}{\left(1 + \frac{B'x_2}{A'x_1}\right)^2}$$

$$\gamma_2 = \exp \left\{ \frac{1,96709}{\left[1 + \frac{1,96709 \cdot (1 - 0,479)}{1,42149 \cdot 0,479}\right]^2} \right\} = 1,36812$$