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:

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

uz parametre:

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

Izračunati koeficijente aktivnosti obiju 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 Laarovom modelu. Konstante van Laarovog 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

γ=?

benzen(1) – *i*-propanol(2)

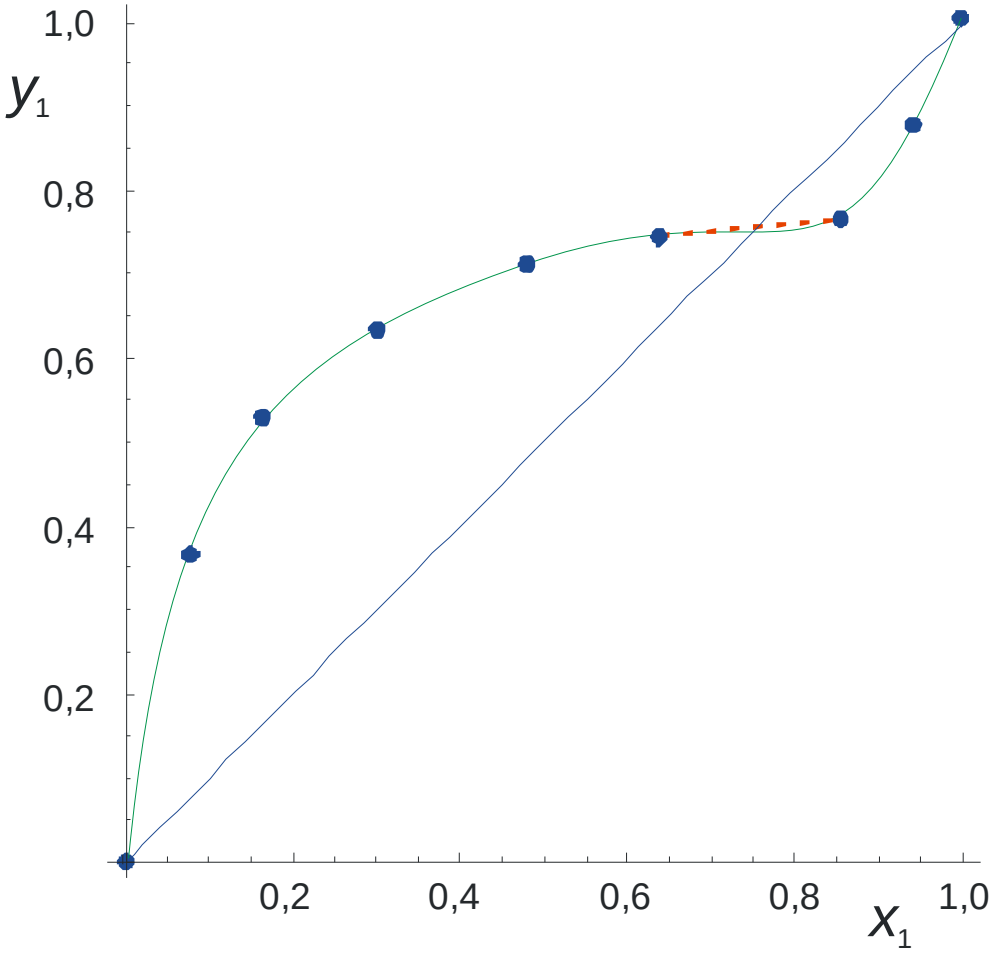
Azeotropna točka, Van Laar

Ravnotežni tlakovi čistih komponenata:

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

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

xy-dijagram

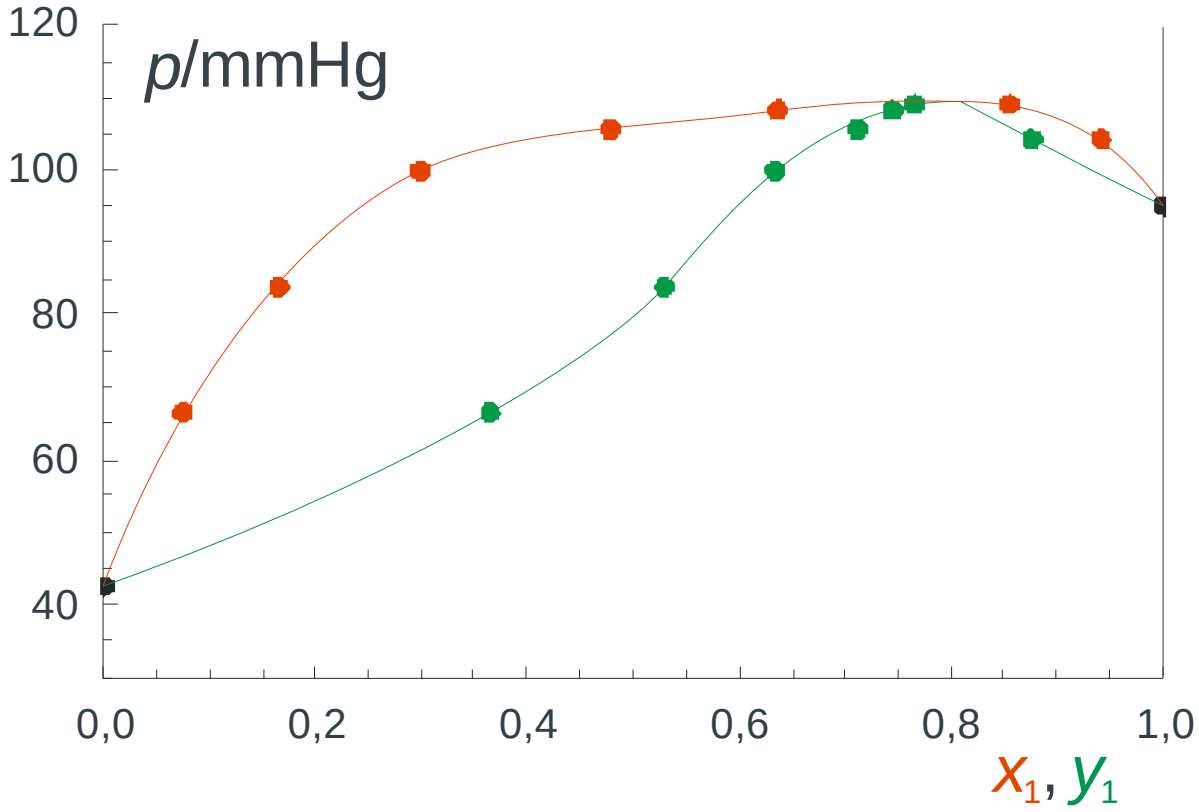


Linearnom interpolacijom:

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

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

Dijagram vrenja:



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

Koeficijenti aktivnosti u azeotropnoj točki!

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

$$p y_i = x_i \gamma_i^L p_i^\bullet$$

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

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

Parametri Van Laarovog modela

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

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

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

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

Koeficijenti aktivnosti preko Van Laarovog modela

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

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

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

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