38. ZADATAK

Za sustav *n*-heksan(1) – 2-butanol(2) određeni su parametri ravnotežnog stanja pri temperaturi od 60 °C:

x_1	0,310	0,607	0,897
y_1	0,779	0,847	0,902
p/mmHg	477,5	563,9	597,0

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
n-heksan(1)	6,87776	1171,530	224,366
2-butanol(2)	7,82863	1482,130	199,970

Treba izračunati prosječne vrijednosti konstanti van Laarovog modela koeficijenta aktivnosti $\overline{A}$ i $\overline{B}$, koristeći sve raspoložive eksperimentalne podatke.

RJEŠENJE

$$\overline{A} = ?$$

$$\overline{B} = ?$$

n-heksan(1) – 2-butanol(2)

Van Laar

Iz Antoineovog izraza:

$$p_1^\bullet = 10^{A_1 - \frac{B_1}{(T/°\mathrm{C}) + C_1}} = 10^{6{,}87776 - \frac{1171{,}530}{60 + 224{,}366}} = 572{,}748\ \mathrm{mmHg}$$

$$p_2^\bullet = 10^{A_2 - \frac{B_2}{(T/°\mathrm{C}) + C_2}} = 10^{7{,}82863 - \frac{1482{,}130}{60 + 199{,}970}} = 134{,}113\ \mathrm{mmHg}$$

$$x_2 = 1 - x_1$$

$$y_2 = 1 - y_1$$

$$\frac{y_\mathrm{i}}{x_\mathrm{i}} = \frac{\gamma_\mathrm{i}^\mathrm{L} p_\mathrm{i}^\bullet}{p} \exp\left[\frac{v_\mathrm{i}^\mathrm{L}\left(p - p_\mathrm{i}^\bullet\right)}{RT}\right] \approx \frac{\gamma_\mathrm{i}^\mathrm{L} p_\mathrm{i}^\bullet}{p}$$

$$p y_\mathrm{i} = x_\mathrm{i} \gamma_\mathrm{i}^\mathrm{L} p_\mathrm{i}^\bullet$$

$$\gamma_1^\mathrm{L} = \frac{y_1 p}{x_1 p_1^\bullet}$$

$$\gamma_2^\mathrm{L} = \frac{y_2 p}{x_2 p_2^\bullet}$$

x_2	0,69	0,393	0,103
y_2	0,221	0,153	0,098
γ_1	2,09501	1,37383	1,04815
γ_2	1,14037	1,63693	4,23537

$$A' = \ln\gamma_1\left(1+\frac{x_2\ln\gamma_2}{x_1\ln\gamma_1}\right)^2$$

$$B' = \ln\gamma_2\left(1+\frac{x_1\ln\gamma_1}{x_2\ln\gamma_2}\right)^2$$

A'	1,43985	1,2763	0,96269
B'	1,63638	1,9622	2,37882

$$\overline{A} = \frac{1{,}43985+1{,}2763+0{,}96269}{3} = 1{,}22628$$

$$\overline{B} = \frac{1{,}63638+1{,}9622+2{,}37882}{3} = 1{,}99247$$

Izračunate se vrijednosti Van Laarovih konstanti mogu primjenjivati za izračunavanje koeficijenata aktivnosti za druge zadane sastave!