

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:

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

uz parametre:

	A	B	C
<i>n</i> -heksan (1)	6,87776	1171,530	224,366
2-butanol (2)	7,82863	1482,130	199,970

Treba izračunati prosječne vrijednosti konstanti van Laarova modela koeficijenta aktiviteta $\bar{A}$ i $\bar{B}$, koristeći se svim raspoloživim eksperimentalnim podacima.

RJEŠENJE

$$\overline{A} = ?$$

$$\overline{B} = ?$$

n-heksan(1) – 2-butanol(2)

Van Laar

Iz Antoineova izraza:

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

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

$$x_2 = 1 - x_1$$

$$y_2 = 1 - y_1$$

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

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

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

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

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

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

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

$$A' \quad 1,43985 \quad 1,2763 \quad 0,96269$$

$$B' \quad 1,63638 \quad 1,9622 \quad 2,37882$$

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

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

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