15. ZADATAK

Procijeniti koeficijente kompresibilnosti i fugacitivnosti ekvimolarne smjese metanola(1), etanola(2) i acetona(3) pri temperaturi od 300 K i tlaku od 8 bar. Pretpostaviti da se plinska smjesa pri tim uvjetima vlada prema Soave-Redlich-Kwongovom modelu.

Pseudokritične parametre smjese izračunati prema Kayevom i Prausnitz-Gunnovom pravilu. Polinomni oblik funkcije, $z=f(z)$, riješiti Newton-Gossetovim postupkom.

Provjeriti fazno područje, odnosno potvrditi stabilnost faza.

Podaci:

	T_K/K	v_K/cm^{3}mol^{-1}	z_K	ω
metanol(1)	512,6	118,0	0,224	0,556
etanol(2)	513,9	167,1	0,240	0,644
aceton(3)	508,1	209,0	0,232	0,304

SOAVE REDLICH KWONG (1972)

Jednadžba

$$p = \frac{RT}{v-b} - \frac{a\alpha}{v(v+b)}$$

$$v^3 - \frac{RT}{p}v^2 - \left(b^2 + \frac{RTb}{p} - \frac{a\alpha}{p}\right)v - \frac{a\alpha b}{p} = 0$$

$$z^3 - z^2 - \left(\frac{b^2p^2}{R^2T^2} + \frac{bp}{RT} - \frac{a\alpha p}{R^2T^2}\right)z - \frac{a\alpha bp^2}{R^3T^3} = 0$$

$$z^3 - z^2 + \left(A - B^2 - B\right)z - AB = 0$$

Parametri

$$a = \frac{\Omega_a R^2 T_\mathrm{k}^2}{p_\mathrm{k}} \qquad b = \frac{\Omega_b R T_\mathrm{k}}{p_\mathrm{k}}$$

$$\Omega_a = \frac{1}{9\left(2^{1/3}-1\right)} = 0{,}427480 \quad \Omega_b = \frac{\left(2^{1/3}-1\right)}{3} = 0{,}086640$$

$$\alpha = \left(1 + \kappa\left(1 - \sqrt{T_\mathrm{r}}\right)\right)^2$$

$$\kappa = 0{,}48508 + 1{,}55171\omega - 0{,}15613\omega^2$$

vodik : $\alpha = 1{,}202\exp\left(-0{,}30288T_\mathrm{r}\right)$

$$A = \frac{a\alpha p}{R^2T^2} = \frac{\Omega_a \alpha p_\mathrm{r}}{T_\mathrm{r}^2} \qquad B = \frac{bp}{RT} = \frac{\Omega_b p_\mathrm{r}}{T_\mathrm{r}}$$

SMJESE REALNIH PLINOVA

Pseudokritični parametri

Kay

$$v_{\mathrm{KM}} = \sum y_{\mathrm{i}} v_{\mathrm{ki}}$$

$$T_{\mathrm{KM}} = \sum y_{\mathrm{i}} T_{\mathrm{ki}}$$

$$p_{\mathrm{KM}} = \sum y_{\mathrm{i}} p_{\mathrm{ki}}$$

Prausnitz i Gunn

$$v_{\mathrm{KM}} = \sum y_{\mathrm{i}} v_{\mathrm{ki}}$$

$$T_{\mathrm{KM}} = \sum y_{\mathrm{i}} T_{\mathrm{ki}}$$

$$z_{\mathrm{KM}} = \sum y_{\mathrm{i}} z_{\mathrm{ki}}$$

$$p_{\mathrm{KM}} = \frac{z_{\mathrm{KM}} R T_{\mathrm{KM}}}{v_{\mathrm{KM}}}$$

Newton-Gosset (SRK)

$$f(z) = z^3 - z^2 + \left(A - B^2 - B\right)z - AB$$

$$f'(z) = 3z^2 - 2z + \left(A - B^2 - B\right)$$

Početne pretpostavke:

$$z^{\mathrm{V}} = 1 \qquad z^{\mathrm{L}} = B$$

Konačna rješenja za koeficijent fugacitivnosti smjese:

$$v^{\mathrm{V}} = \frac{z^{\mathrm{V}}RT}{p} = \frac{0,9467 \cdot 8,314 \cdot 273,2}{101325} = 2,1222 \cdot 10^{-2}\,\mathrm{m^3mol^{-1}}$$

$$\ln \varphi^{\mathrm{V}} = \ln \frac{v^{\mathrm{V}}}{v^{\mathrm{V}} - b} + \frac{a\alpha(T)}{bRT} \ln \frac{v^{\mathrm{V}}}{v^{\mathrm{V}} + b} + \left(z^{\mathrm{V}} - 1\right) - \ln z^{\mathrm{V}}$$

$$v^{\mathrm{L}} = \frac{z^{\mathrm{L}}RT}{p} = \frac{5,46066 \cdot 10^{-3} \cdot 8,314 \cdot 273,2}{101325} = 1,22411 \cdot 10^{-4}\,\mathrm{m^3mol^{-1}}$$

$$\ln \varphi^{\mathrm{L}} = \ln \frac{v^{\mathrm{L}}}{v^{\mathrm{L}} - b} + \frac{a\alpha(T)}{bRT} \ln \frac{v^{\mathrm{L}}}{v^{\mathrm{L}} + b} + \left(z^{\mathrm{L}} - 1\right) - \ln z^{\mathrm{L}}$$

Parcijalne fugacitivnosti komponenata:

$$\ln \hat{\varphi}_{\mathrm{i}} = \frac{b_{\mathrm{i}}}{b_{\mathrm{M}}}(z-1) - \ln\left[z\left(1-\frac{b_{\mathrm{M}}}{v}\right)\right] + \frac{1}{b_{\mathrm{M}}RT}\left(\frac{(a\alpha)_{\mathrm{M}} b_{\mathrm{i}}}{b_{\mathrm{M}}} - 2\sum_{\mathrm{j}} y_{\mathrm{j}}(a\alpha)_{\mathrm{ij}}\right)\ln\left(1+\frac{b_{\mathrm{M}}}{v}\right)$$

TREBA TESTIRATI PARCIJALNE FUGACITIVNOSTI KOMPONENATA.

Može se dogoditi da je parcijalna fugacitivnost za jednu komponentu viša u parnoj, a za drugu u kapljevitoj fazi. Uspostavlja se fazna ravnoteža para-kapljevina s različitim sastavima parne i kapljevite faze! Problem stabilnosti rješava se na drugačiji način nego za čistu komponentu!