11. ZADATAK

Procijeniti koeficijent kompresibilnosti i molarni volumen ekvimolarne smjese CO_2 i etana pri temperaturi od 250 K i tlaku od 10 atm. Pretpostaviti da se plinska smjesa pri tim uvjetima vlada prema Soave-Redlich-Kwongovom modelu.

Parametre smjese izračunati primjenom pravila miješanja, a polinomni oblik funkcije, $z=f(z)$, riješiti Newton-Gossetovim postupkom.

Podaci:

	T_K/K	p_K/atm	ω
CO_2(1)	304,2	73,8	0,225
etan(2)	305,4	48,8	0,099

unakrsni parametri: $k_{12}=k_{21}=0,1$

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

Pravila miješanja
Soave-Redlich-Kwong

$$\left(a\alpha\right)_{\mathrm{M}} = \sum_i \sum_j y_i y_j \left(aa\right)_{ij}$$

$$b_{\mathrm{M}} = \sum_i y_i b_i$$

$$A_{\mathrm{M}} = \sum_i \sum_j y_i y_j A_{ij}$$

$$B_{\mathrm{M}} = \sum_i y_i B_i$$

Dvokomponentne smjese

$$\left(a\alpha\right)_{\mathrm{M}} = \left(a\alpha\right)_{11} y_1^2 + \left(a\alpha\right)_{12} y_1 y_2 + \left(a\alpha\right)_{21} y_2 y_1 + \left(a\alpha\right)_{22} y_2^2 =$$

$$= \left(a\alpha\right)_1 y_1^2 + 2\left(a\alpha\right)_{12} y_1 y_2 + \left(a\alpha\right)_2 y_2^2$$

$$\left(a\alpha\right)_{11} = \left(a\alpha\right)_1 \quad \left(a\alpha\right)_{22} = \left(a\alpha\right)_2 \quad \left(a\alpha\right)_{12} = \left(a\alpha\right)_{21}$$

$$b_{\mathrm{M}} = b_1 y_1 + b_2 y_2$$

Unakrsni parametri

Soave Redlich Kwong

$$\left(a\alpha\right)_{12} = \left(1 - k_{12}\right)\sqrt{\left(a\alpha\right)_1 \left(a\alpha\right)_2}$$

Zadatak:

$CO_2(1)$ – ETAN(2)

$T = 250\ \text{K}$

$p = 10\ \text{atm} = 1{,}013250\ \text{MPa}$

$y_1 = 0{,}5$

Parametri *a* i *b* pojedinačnih fluida

$$a_1 = \frac{\Omega_a R^2 T_{\text{K1}}^2}{p_{\text{K1}}} = \frac{0{,}42748 \cdot 8{,}314^2 \cdot 304{,}2^2}{73{,}8 \cdot 101325} = 0{,}3657$$

$$b_1 = \frac{\Omega_b R T_{\text{K1}}}{p_{\text{K1}}} = \frac{0{,}08664 \cdot 8{,}314 \cdot 304{,}2}{73{,}8 \cdot 101325} = 2{,}93 \cdot 10^{-5}$$

$$a_2 = \frac{\Omega_a R^2 T_{\text{K2}}^2}{p_{\text{K2}}} = \frac{0{,}42748 \cdot 8{,}314^2 \cdot 305{,}4^2}{48{,}8 \cdot 101325} = 0{,}5574$$

$$b_2 = \frac{\Omega_b R T_{\text{K2}}}{p_{\text{K2}}} = \frac{0{,}08664 \cdot 8{,}314 \cdot 305{,}4}{48{,}8 \cdot 101325} = 4{,}449 \cdot 10^{-5}$$

Reducirane temperature pojedinačnih fluida

$$T_{\text{r1}} = \frac{T}{T_{K1}} = \frac{250}{304{,}2} = 0{,}8218 \qquad T_{\text{r2}} = \frac{T}{T_{K2}} = \frac{250}{305{,}4} = 0{,}8186$$

Parametri κ pojedinačnih fluida

$$\kappa_1 = \left(0,48508 + 1,55171\omega_1 - 0,15613\omega_1^2\right) =$$
$$= \left(0,48508 + 1,55171 \cdot 0,225 - 0,15613 \cdot 0,225^2\right) =$$
$$= 0,826311$$

$$\kappa_2 = \left(0,48508 + 1,55171\omega_2 - 0,15613\omega_2^2\right) =$$
$$= \left(0,48508 + 1,55171 \cdot 0,099 - 0,15613 \cdot 0,099^2\right) =$$
$$= 0,637169$$

Parametri α pojedinačnih fluida

$$\alpha_1 = \left[1 + \kappa_1\left(1 - \sqrt{T_{r1}}\right)\right]^2 =$$
$$= \left[1 + 0,826311\left(1 - \sqrt{0,8218}\right)\right]^2 = 1,1604$$

$$\alpha_2 = \left[1 + \kappa_2\left(1 - \sqrt{T_{r2}}\right)\right]^2 =$$
$$= \left[1 + 0,637169\left(1 - \sqrt{0,8186}\right)\right]^2 = 1,1247$$

Pravila miješanja

$$(a\alpha)_{11} = 0,3657 \cdot 1,1604 = 0,4244$$
$$(a\alpha)_{22} = 0,5574 \cdot 1,1247 = 0,6269$$
$$(a\alpha)_{12} = (1 - k_{12})\sqrt{(a\alpha)_1 (a\alpha)_2} =$$
$$= (1 - 0,1)\sqrt{0,4244 \cdot 0,6269} = 0,4642$$

$$(a\alpha)_{\mathrm{M}} = \sum_i \sum_j y_i y_j (a\alpha)_{ij} =$$

$$= y_1^2 (a\alpha)_{11} + 2 y_1 y_2 (a\alpha)_{12} + y_2^2 (a\alpha)_{22} =$$

$$= 0,5^2 \cdot 0,4244 + 2 \cdot 0,5 \cdot 0,5 \cdot 0,4642 + 0,5^2 \cdot 0,6269 =$$

$$= 0,4949$$

$$b_{\mathrm{M}} = \sum_i y_i b_i =$$

$$= y_1 b_1 + y_2 b_2 = 0,5 \cdot 2,93 \cdot 10^{-5} + 0,5 \cdot 4,449 \cdot 10^{-5} =$$

$$= 3,6895 \cdot 10^{-5}$$

Parametri A i B smjese

$$A = \frac{(a\alpha)_{\mathrm{M}}\, p}{R^2 T^2} = \frac{0,4949 \cdot 1013250}{8,314^2 \cdot 250^2} = 0,1160$$

$$B = \frac{b_{\mathrm{M}}\, p}{R^2 T^2} = \frac{3,6895 \cdot 10^{-5} \cdot 1013250}{8,314 \cdot 250} = 0,0180$$

Newton-Gosset (SRK)

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

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

Početne pretpostavke:

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

$$z^{(0)}=1 \qquad z^{(0)}=0{,}018$$

$$z^{(1)}=0{,}912918 \qquad z^{(1)}=0{,}0283435$$

$$z^{(2)}=0{,}89413 \qquad z^{(2)}=0{,}0306501$$

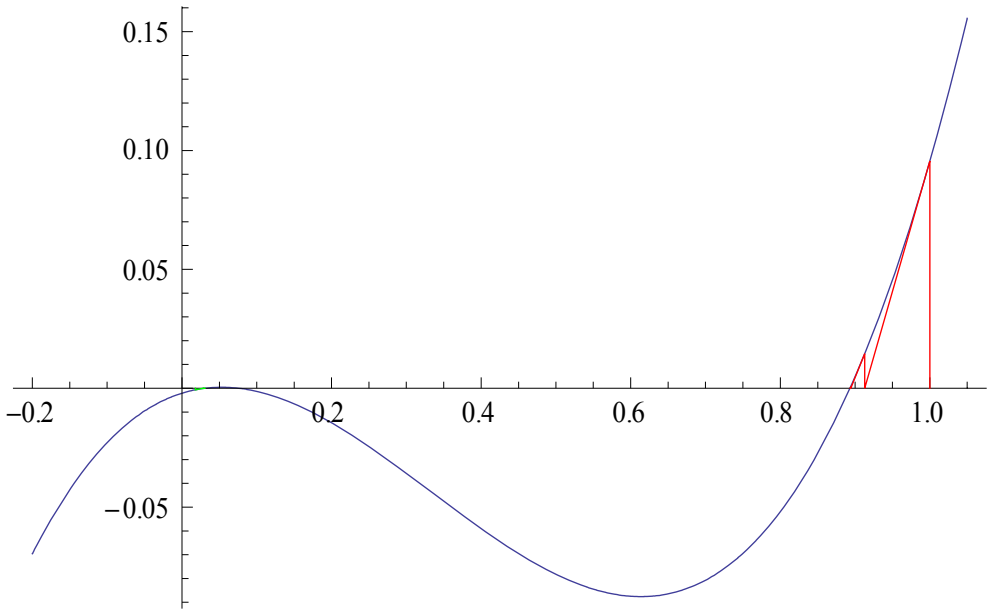
$$z^{(3)}=0{,}893272 \qquad z^{(3)}=0{,}030774$$

$$z^{(4)}=0{,}89327 \qquad z^{(4)}=0{,}0307744$$

$$z^{(5)}=0{,}89327 \qquad z^{(5)}=0{,}0307744$$

$$v^{\mathrm{V}}=\frac{z^{\mathrm{V}}RT}{p}=\frac{0{,}89327\cdot 8{,}314\cdot 250}{1013250}=1{,}83238\cdot 10^{-3}\,\mathrm{m^3mol^{-1}}$$

$$v^{\mathrm{L}}=\frac{z^{\mathrm{L}}RT}{p}=\frac{0{,}0307744\cdot 8{,}314\cdot 250}{1013250}=6{,}31281\cdot 10^{-5}\,\mathrm{m^3mol^{-1}}$$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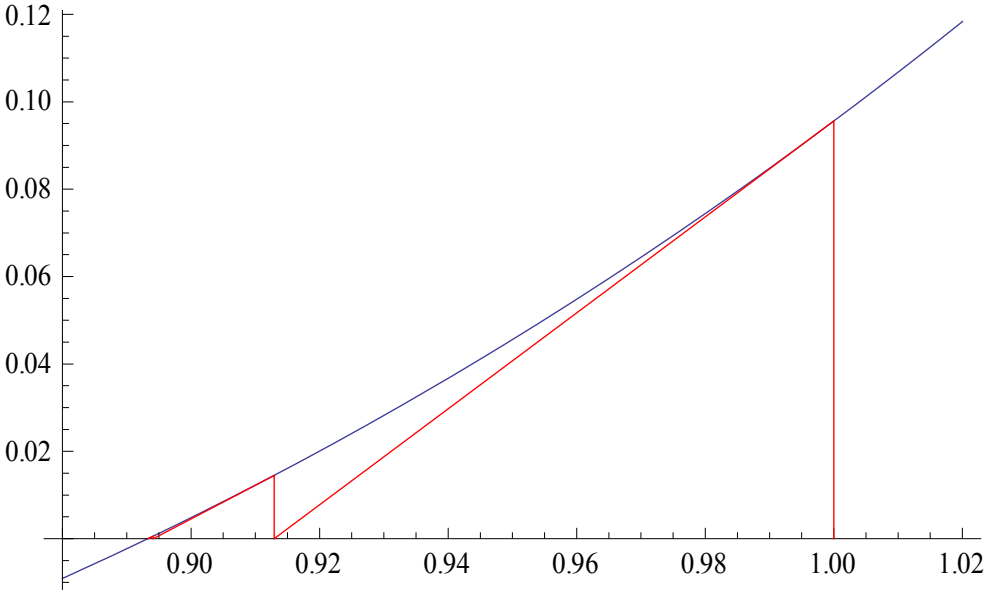
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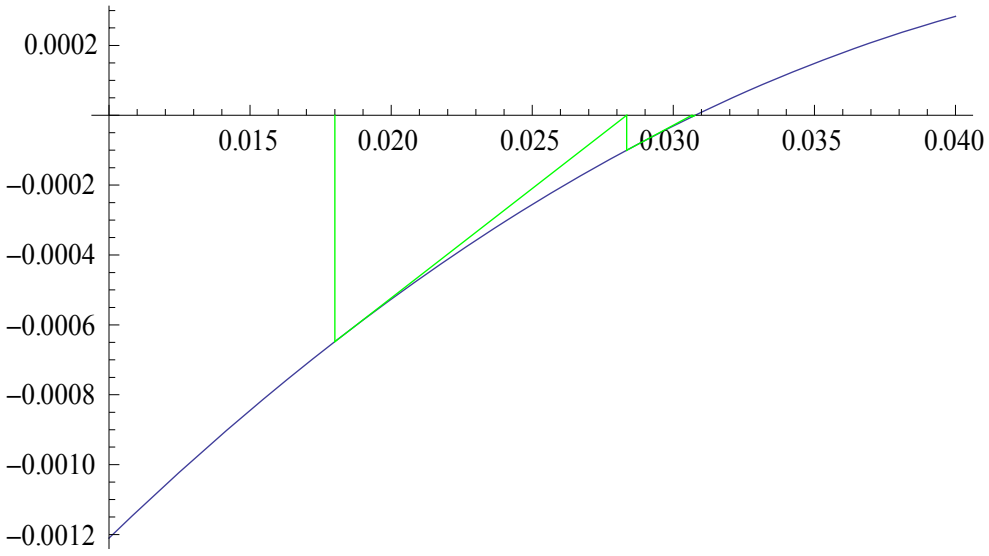
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