# 11. ZADATAK

Procijeniti faktor 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-Kwongovu 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 | $\omega$ |
|---|---|---|---|
| $CO_2(1)$ | 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**

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

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

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

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

**Parametri**

$$a = \frac{\Omega_a R^2 T_k^2}{p_k} \qquad\qquad b = \frac{\Omega_b RT_k}{p_k}$$

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

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

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

**vodik :** $\quad \alpha = 1,202 \exp\left(-0,30288 T_r\right)$

$$A = \frac{a\alpha p}{R^2 T^2} = \frac{\Omega_a \alpha p_r}{T_r^2} \qquad\qquad B = \frac{bp}{RT} = \frac{\Omega_b p_r}{T_r}$$

# SMJESE REALNIH PLINOVA

**Pravila miješanja**
**Soave-Redlich-Kwong**

$$(a\alpha)_M = \sum_i \sum_j y_i y_j (aa)_{ij}$$

$$b_M = \sum_i y_i b_i$$

$$A_M = \sum_i \sum_j y_i y_j A_{ij}$$

$$B_M = \sum_i y_i B_i$$

**Dvokomponentne smjese**

$$(a\alpha)_M = (a\alpha)_{11} y_1^2 + (a\alpha)_{12} y_1 y_2 + (a\alpha)_{21} y_2 y_1 + (a\alpha)_{22} y_2^2 =$$
$$= (a\alpha)_1 y_1^2 + 2(a\alpha)_{12} y_1 y_2 + (a\alpha)_2 y_2^2$$
$$(a\alpha)_{11} = (a\alpha)_1 \quad (a\alpha)_{22} = (a\alpha)_2 \quad (a\alpha)_{12} = (a\alpha)_{21}$$

$$b_M = b_1 y_1 + b_2 y_2$$

**Unakrsni parametri**

**Soave Redlich Kwong**

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

Zadatak:

$CO_2$ (1) – ETAN (2)

$T = 250$ K

$p = 10$ atm=1,013250 MPa

$y_1 = 0,5$

Parametri $a$ i $b$ pojedinačnih fluida

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

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

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

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

Reducirane temperature pojedinačnih fluida

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

Parametri $\kappa$ 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 $\alpha$ 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

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

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

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

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

$$= 0,4949$$

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

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

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

Parametri $A$ i $B$ smjese

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

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

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:

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

| | |
|---|---|
| $z^{(0)}=1$ | $z^{(0)}=0{,}018$ |
| $z^{(1)}=0{,}912918$ | $z^{(1)}=0{,}0283435$ |
| $z^{(2)}=0{,}89413$ | $z^{(2)}=0{,}0306501$ |
| $z^{(3)}=0{,}893272$ | $z^{(3)}=0{,}030774$ |
| $z^{(4)}=0{,}89327$ | $z^{(4)}=0{,}0307744$ |
| $z^{(5)}=0{,}89327$ | $z^{(5)}=0{,}0307744$ |

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

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