7. ZADATAK

Izračunati koeficijent fugacitivnosti *n*-pentana pri temperaturi od 273,2 K i tlaku od 1 atm. Pretpostaviti da se pentan pri tim uvjetima vlada prema Soave-Redlich-Kwongovom modelu.

Koeficijent kompresibilnosti izračunati Newton-Gossetovim postupkom, u skladu sa Soave-Redlich-Kwongovom jednadžbom, iskazanom u polinomnom obliku, $z=f(z)$.

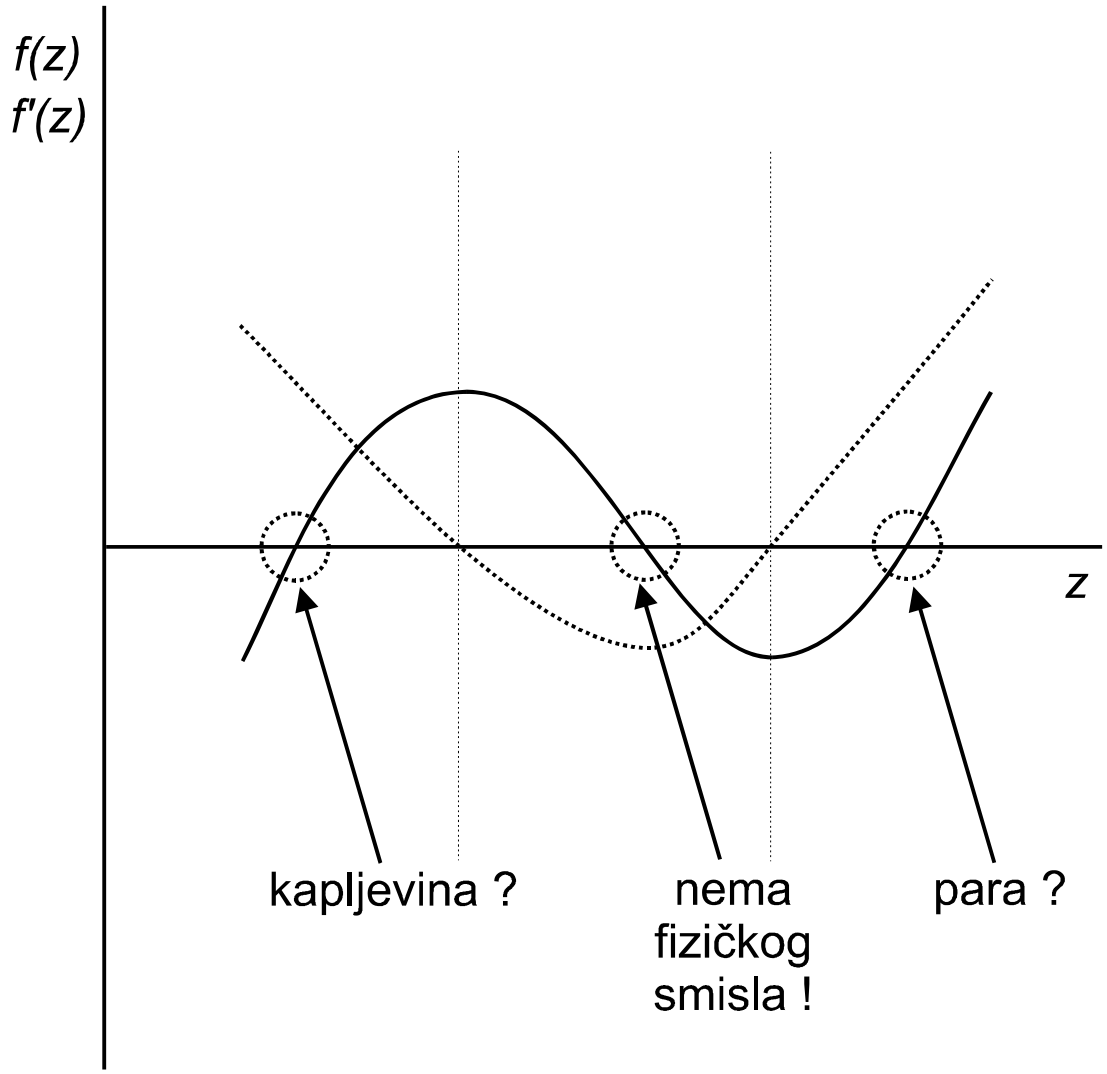
Podaci:

T_K=469,7 K; p_K=33,7 bara; ω=0,251

GOSSET NEWTON METODA (1986)

Jednadžbe stanja trećeg stupnja po *z*
(Soave Redlich Kwong)

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



Zadatak:

$$p = 1\ \text{atm} = 101325\ \text{Pa}$$

$$T = 273,2\ \text{K}$$

Jednadžba stanja trećeg stupnja

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

Parametri:

$$a = \frac{\Omega_a R^2 T_\text{K}^2}{p_\text{K}} = \frac{0,427480 \cdot 8,314^2 \cdot 469,7^2}{33,7 \cdot 100000} = 1,9344$$

$$b = \frac{\Omega_b R T_\text{K}}{p_\text{K}} = \frac{0,086640 \cdot 8,314 \cdot 469,7}{33,7 \cdot 100000} = 1,004 \cdot 10^{-4}$$

$$T_\text{r} = T/T_\text{K} = 273,2/469,7 = 0,581861$$

$$\kappa = 0,48508 + 1,55171\omega - 0,1561\omega^2 =$$

$$= 0,48508 + 1,55171 \cdot 0,251 - 0,1561 \cdot 0,251^2 =$$

$$= 0,8647$$

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

$$= \left[1 + 0,8647\left(1 - \sqrt{0,581861_\text{r}}\right)\right]^2 = 1,4526$$

$$A = \frac{a\alpha p}{R^2 T^2} = \frac{1,9344 \cdot 1,4526 \cdot 101325}{8,314^2 \cdot 273,2^2} = 0,0552$$

$$B = \frac{bp}{RT} = \frac{1,004 \cdot 10^{-4} \cdot 101325}{8,314 \cdot 273,2} = 4,4788 \cdot 10^{-3}$$

Proračun parne faze:

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

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

$$f(z) = 0$$

$$z^{(i+1)} = z^{(i)} - \frac{f(z^{(i)})}{f'(z^{(i)})}$$

Prva aproksimacija – idealni plin:

$$z^{(0)} = \frac{pv}{RT} = 1$$

$$f(z^{(0)}) = 1^3 - 1^2 + (0,0552 - (4,4788 \cdot 10^{-3})^2 - 4,4788 \cdot 10^{-3})1 - 0,0552 \cdot 4,4788 \cdot 10^{-3} = 0,0504$$

$$f'(z^{(0)}) = 3 \cdot 1^2 - 2 \cdot 1 + (0,0552 - (4,4788 \cdot 10^{-3})^2 - 4,4788 \cdot 10^{-3}) = 1,0507$$

$$z^{(1)} = z^{(0)} - \frac{f(z^{(0)})}{f'(z^{(0)})} = 1 - \frac{0,0504}{1,0507} = 0,9520$$

$$f(z^{(1)}) = 0,9520^3 - 0,9520^2 + (0,0507)0,9520 - 2,472 \cdot 10^{-4} = 4,516 \cdot 10^{-4}$$

$$f'(z^{(1)}) = 3 \cdot 0,9520^2 - 2 \cdot 0,9520 + (0,0507) = 0,7351$$

$$z^{(2)} = z^{(1)} - \frac{f(z^{(1)})}{f'(z^{(1)})} = 0,9520 - \frac{4,516 \cdot 10^{-4}}{0,7351} = 0,9514$$

$$z^{(5)} = 0,9467$$

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

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

$$\ln\varphi^{\mathrm{V}} = \ln\frac{2{,}1222\cdot10^{-2}}{2{,}1222\cdot10^{-2}-1{,}004\cdot10^{-4}} +$$

$$+\frac{1{,}9344\cdot1{,}4526}{1{,}004\cdot10^{-4}\cdot8{,}314\cdot273{,}2}\ln\frac{2{,}1222\cdot10^{-2}}{2{,}1222\cdot10^{-2}+1{,}004\cdot10^{-4}} +$$

$$+\left(0{,}9467-1\right) - \ln 0{,}9467$$

$$\ln\varphi^{\mathrm{V}} = 0{,}00474217 +$$

$$+12{,}3216\cdot\left(-0{,}00471978\right) +$$

$$+\left(0{,}9467-1\right) - \ln 0{,}9467$$

$$\ln\varphi^{\mathrm{V}} = -0{,}05194$$

$$\varphi^{\mathrm{V}} = 0{,}949386$$

Proračun kapljevite faze:

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

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

$$f(z) = 0$$

$$z^{(i+1)} = z^{(i)} - \frac{f\left(z^{(i)}\right)}{f'\left(z^{(i)}\right)}$$

Prva aproksimacija – reducirani volumen čestica:

$$z^{(0)} = B = \frac{b}{v^{\mathrm{id}}} = \frac{bp}{RT} = 4,4788 \cdot 10^{-3}$$

$$f\left(z^{(0)}\right) = \left(4,4788 \cdot 10^{-3}\right)^3 - \left(4,4788 \cdot 10^{-3}\right)^2 + (0,0507)\,4,4788 \cdot 10^{-3} - 2,472 \cdot 10^{-4} = -4,0095 \cdot 10^{-5}$$

$$f'\left(z^{(0)}\right) = \left(3 \cdot 4,4788 \cdot 10^{-3}\right)^2 - 2 \cdot 4,4788 \cdot 10^{-3} + (0,0507) = 0,0418$$

$$z^{(1)} = z^{(0)} - \frac{f\left(z^{(0)}\right)}{f'\left(z^{(0)}\right)} = 4,4788 \cdot 10^{-3} - \frac{-4,0095 \cdot 10^{-5}}{0,0418} = 5,438 \cdot 10^{-3}$$

$$z^{(5)} = 5,46066 \cdot 10^{-3}$$

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

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

$$\ln\varphi^{\mathrm{L}} = \ln\frac{1{,}22411\cdot10^{-4}}{1{,}22411\cdot10^{-4}-1{,}004\cdot10^{-4}} +$$

$$+\frac{1{,}9344\cdot1{,}4526}{1{,}004\cdot10^{-4}\cdot8{,}314\cdot273{,}2}\ln\frac{1{,}22411\cdot10^{-4}}{1{,}22411\cdot10^{-4}+1{,}004\cdot10^{-4}} +$$

$$+\left(5{,}46066\cdot10^{-3}-1\right) - \ln 5{,}46066\cdot10^{-3}$$

$$\ln\varphi^{\mathrm{L}} = 1{,}71584 +$$

$$+12{,}3216\cdot\left(-0{,}59894\right) +$$

$$+\left(5{,}46066\cdot10^{-3}-1\right) - \ln 5{,}46066\cdot10^{-3}$$

$$\ln\varphi^{\mathrm{L}} = -1{,}44841$$

$$\varphi^{\mathrm{L}} = 0{,}234943$$

$$\varphi^{\mathrm{V}} \geq \varphi^{\mathrm{L}}$$

Stabilna faza je kapljevina!!

Normalno vrelište pentana: 36,1 °C